Multi-Material Analysis of Layered Hybrid Organic-Inorganic Perovskites

Independent Study Final Project Report

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1 Introduction

Layered hybrid organic-inorganic perovskites (HOIPs) have emerged as a significant class of materials exhibiting remarkable structural versatility and functional properties. Of particular interest is their potential for applications spanning photovoltaics, light-emitting devices, and spintronic technologies [2, 3]. The fundamental architecture of these materials comprises alternating organic and inorganic layers, where the organic components serve as templating agents that influence the structural configuration of the inorganic framework through hydrogen bonding interactions [4].

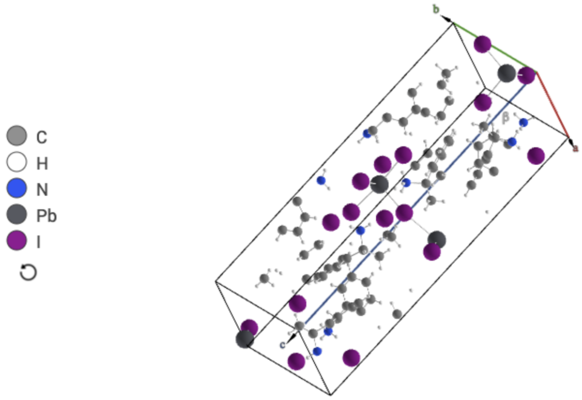


Figure 1: Example of a pre - H relaxed Material Structure

One of the most critical aspects of these systems is the hydrogen bonding network that forms between the organic ammonium groups and the inorganic framework. These interactions play a dual role: they not only stabilize the overall structure but also induce subtle structural distortions that significantly impact the material's electronic and optical properties [1]. The precise nature of these hydrogen bonds, particularly their strength and directionality, can substantially influence the symmetry of the inorganic framework and consequently affect properties such as charge transport, optical absorption, and spin polarization [5].

Research Problem: The Challenge of Accurate Hydrogen Bond Modeling

A significant challenge in studying layered perovskites lies in accurately determining hydrogen atom positions within the structure. As seen in Yi's work on hybrid organic-inorganic perovskites (HOIPs), conventional techniques like X-ray diffraction are limited in capturing precise hydrogen locations due to their low electron density and weak scattering power compared to heavier atoms [1]. This limitation can lead to discrepancies in bond lengths and angles, especially in the hydrogen bonds bridging the organic and inorganic layers, which in turn affects the interpretation of structural symmetry and stability within the material.

Hydrogen bond orientations influence the symmetry of the inorganic framework, and even minor inaccuracies can result in incorrect assumptions about the material's performance in applications such as spintronics and optoelectronics. To overcome these challenges, Yi's research demonstrates the potential of Density Functional Theory (DFT) to refine hydrogen positions within perovskites, especially when experimental hydrogen positions are corrected using "H-only DFT relaxation," which focuses on relaxing hydrogen atoms while maintaining other structural components as fixed [1].

To explore the effects of hydrogen relaxation in different materials, the Density Functional Theory (DFT) is applied at three computational precision levels—light, intermediate, and tight. Each setting allows us to observe changes in hydrogen bond placement, symmetry, and structural distortions, giving insight into the role hydrogen bonds play in perovskite properties. The study also examines how different levels of computational accuracy influence the structural predictions and how refining hydrogen positions affects overall stability. This study uses high-level DFT calculations across these precision levels, alongside a detailed analysis of structural parameters and hydrogen bonding, helping us see how computational choices impact structural and bonding insights in perovskites.

The results of this study contribute to the broader understanding of structure-property relationships in HOIPs and provide insights into more accurate hydrogen bond modeling methodologies for future research.

2 Materials and Methods

2.1 Material Selection

Materials for this study were chosen from the Hybrid3 database, a widely used repository of hybrid organic-inorganic perovskite structures, the selection process prioritized materials with clean and well-defined structures to ensure accurate computational modeling and analysis.

Each candidate material's structure was carefully reviewed by examining its CIF file and corresponding `geometry.in` file. To identify potential structural disorders, CIF files were searched for specific indicators, such as the presence of `uani 0`. If disorder was detected, the material was excluded, and a new candidate was selected. This iterative process helped build a dataset of materials with robust structural integrity, avoiding inaccuracies introduced by disordered structures.

Besides the disorders, the selected materials exhibited somewhat similar patterns, such as analogous hydrogen bonding networks or comparable organic and inorganic frameworks. This approach ensured the dataset would allow meaningful comparisons while still providing enough diversity to explore variations in properties.

In total, 20 materials were selected, representing a balance of structural consistency and variation. This curated collection forms the basis for a detailed computational study of structure-property relationships in hybrid organic-inorganic perovskites.

2.2 Computational Approach

The computational analysis for this study was carried out using a combination of high-performance computing resources, primarily Duke University's Timewarp computational cluster and NERSC's Perlmutter supercomputer. While both systems were utilized, the majority of the computations were performed on Timewarp, leveraging its compatibility and efficiency for the specific requirements of this study.

2.3 Preparation of Input Files

1. Structure Definition: The crystal structure was defined using a geometry.in file or a CIF file containing initial atomic positions and lattice parameters specific to the chosen compound. If a CIF file was given it was converted to the necessary input format (geometry.in) for FHI-aims.

2. Control File Setup: A `control.in` file was created to specify computational parameters for each relaxation setting:

    - Light Setting: Applies moderate precision to adjust hydrogen positions and gain an overall view of the bonding network.
    - Intermediate Setting: Uses higher accuracy to build on the light setting, revealing finer structural details.
    - Tight Setting: Employs the highest precision and strictest criteria to uncover tiny distortions and slight symmetry breaks within the structure.

3. **Species Defaults:** Species-specific parameters were added to `control.in` for elements (eg. Pb, I, C, H, N) in the compound. These files were defaulted using `$SPECIES_DEFAULTS`, including tight settings for heavier elements to enhance the accuracy of electronic structure and bonding calculations.

2.4 Execution of Calculations

The calculations were primarily executed on Timewarp, which provided robust support for large-scale DFT computations. Selected computations, particularly those requiring enhanced scalability, were also run on Perlmutter to take advantage of its GPU-accelerated architecture. Both systems were instrumental in ensuring computational efficiency and accuracy.

1. Light Setting Relaxation: This first run aimed to establish a stable geometry with moderate precision, offering a broad view of bond lengths, bond angles, and key estimated properties.
2. Intermediate Setting Relaxation: This stage enhanced hydrogen positioning accuracy and reduced atomic forces further, refining initial observations and preparing the structure for the final, highest-precision run.
3. Tight Setting Relaxation: Finally, the tight setting was employed to achieve maximum precision in hydrogen placement and structural symmetry. This setting offered the most accurate insights into subtle distortions and hydrogen bond behavior.

Each job was monitored using `squeue`. Relevant output files, including `aims.out` were collected for further analysis.

Post-Processing and Data Analysis

For each setting, the results were analyzed for Total energy, Fermi energy, Highest occupied and lowest unoccupied states, Cell volume and Structural metrics (bond lengths, angles, and symmetry characteristics), bond length difference and more.

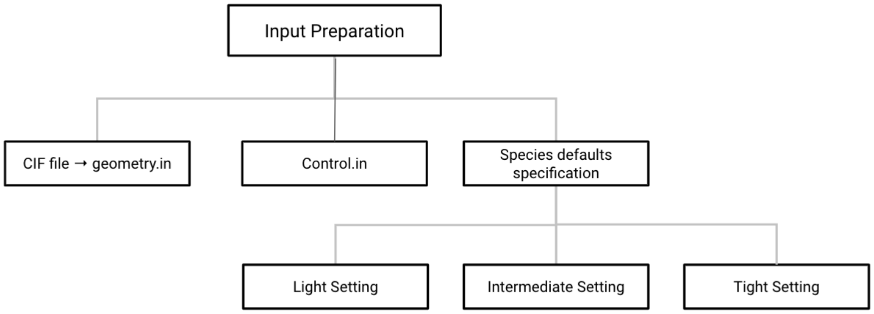


Figure 2: Approach to the analysis

3 Results

3.1 Material 3: 5,5“‘-bis(aminoethyl)-2,2‘:5‘,2“:5“,2“‘-quaterthiophene lead bromide

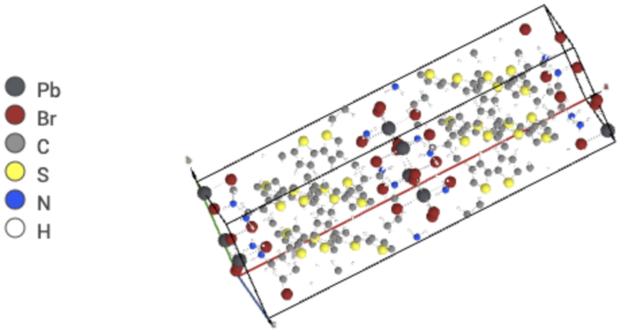


Figure 3: Tight setting rendition of the material

The analysis for this material was conducted after relaxation at intermediate settings. It was analyzed using 16 parallel tasks over 27635.890s, requiring 4933.383 MB peak memory. The structure (424 atoms, cell volume 5369.18 Å^3) shows a HOMO-LUMO gap of 1.81 eV. The relaxation process exited without errors, confirming proper convergence.

Hydrogen Movement Analysis
With an average displacement of 0.098 Å ($\sigma = 0.075$ Å) and a mean bond length change of 0.035 Å. The final average bond length across all hydrogen atoms was 1.327 Å. The analysis identified four distinct bond types:

- **H-C:** Average bond length = 1.145 Å (112 bonds, forming the backbone of the structure),
- **H-N:** Average bond length = 1.020 Å (42 bonds, contributing significantly to structural stabilization),
- **H-Br:** Average bond length = 2.684 Å (4 bonds, indicative of weak hydrogen-halide interactions),
- **H-H:** Average bond length = 2.533 Å (18 bonds, representing secondary structural features).

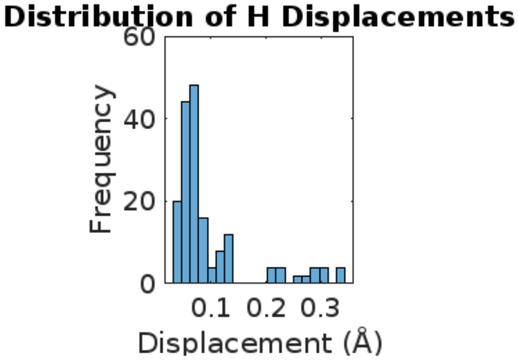


Figure 4: Bimodal H displacement distribution.

Movement Analysis of Key Groups
The hydrogen displacements were grouped into two main categories based on bond type and movement patterns:

1. **N-H Bonds (H420-H388):**
    - Average displacement = 0.342 Å,
    - Average bond length change = 0.023 Å,
    - Final bond length = 1.043 Å.

   These movements underscore the critical role of N-H bonds in stabilizing the material's organic-inorganic framework.

2. **Mixed Bonds (H377-H379):**
    - Average displacement = 0.298 Å,
    - Average bond length change = 0.111 Å,
    - Final bond length = 2.038 Å.

   This group includes a combination of N-H and H-H bonds, where larger bond length changes suggest potential rearrangements in hydrogen bonding during relaxation.

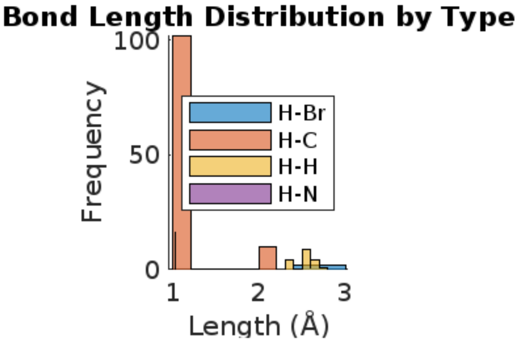
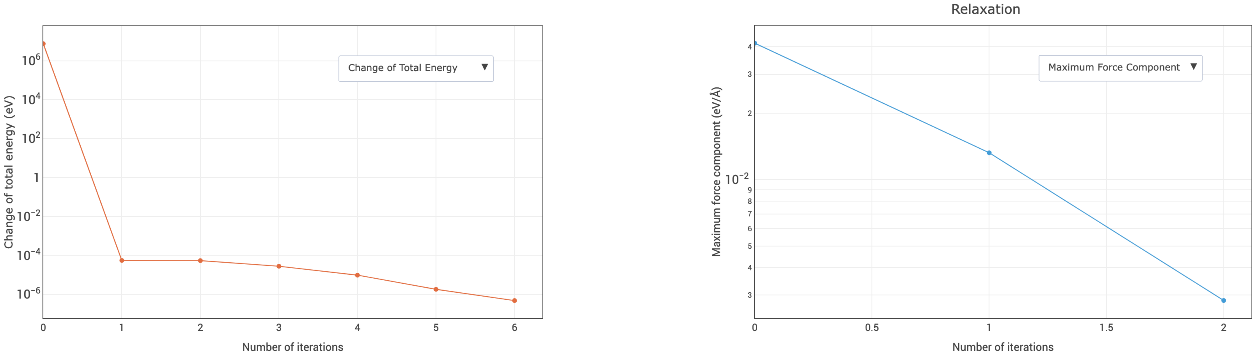


Figure 5: Bond type distribution.

Convergence Behavior

The energy convergence analysis demonstrates a systematic decrease in total energy, stabilizing to within 10^{-5} eV across six iterations. Similarly, the force convergence shows a steady reduction, with the maximum force component decreasing to below 10^{-2} eV/Å by the final step. These trends confirm the reliability of the relaxation process and the suitability of intermediate settings for capturing key structural dynamics.



(a) Energy convergence during relaxation.

(b) Force convergence during relaxation.

Figure 6: Convergence behavior of Material 3 showing energy and force stabilization over iterations.

Correlation Analysis

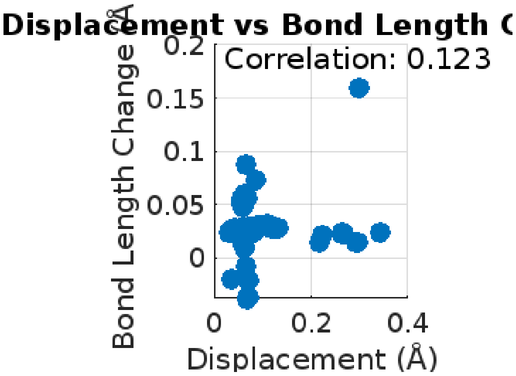


Figure 7: Bond type distribution.

The weak correlation coefficient of 0.123 between hydrogen displacement and bond length changes suggests largely independent mechanisms of structural relaxation. This independence highlights the complex interplay between hydrogen movements and the overall framework stability, where localized adjustments do not directly translate into proportional bond length modifications.

3.2 Material 7: Bis(1-(2-naphthyl)methylammonium) lead bromide

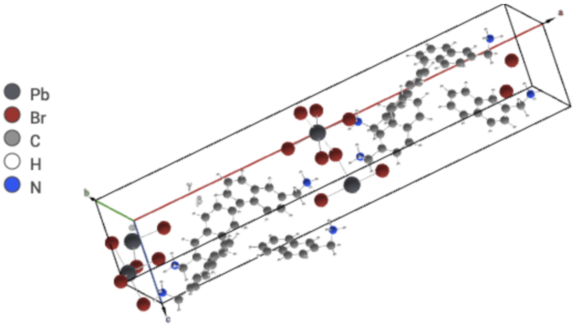


Figure 8: Tight setting rendition of the material

The analysis for this material was conducted after relaxation at tight settings. It was analyzed using 60 parallel tasks over 19533.608s, requiring 1305.865 MB peak memory. The structure (212 atoms, cell volume 2630.37 Å^3) shows a HOMO-LUMO gap of 2.57 eV. The relaxation process exited without errors, confirming proper convergence.

Hydrogen Movement Analysis
With an average displacement of 0.000124 Å ($\sigma = 0.000093$ Å) and a mean bond length change of 0.000003 Å, the final average bond length across all hydrogen atoms was 1.079419 Å. The analysis identified two distinct bond types:

- **H-C:** Average bond length = 1.091394 Å (72 bonds, forming the backbone of the structure),
- **H-N:** Average bond length = 1.043482 Å (24 bonds, contributing significantly to structural stabilization).

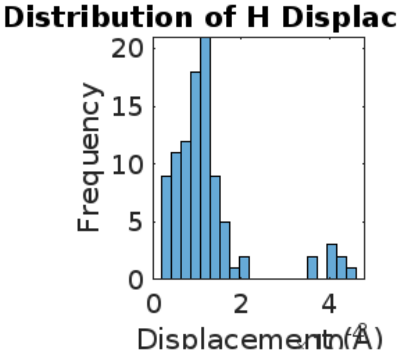


Figure 9: Bimodal H displacement distribution.

Movement Analysis of Key Groups
The hydrogen displacements were grouped into two main categories based on bond type and movement patterns:

1. **H159-H49 Group:**
    - Average displacement = 0.000362 Å,
    - Average bond length change = -0.000007 Å,
    - Final bond length = 1.086169 Å.

This group includes predominantly H-C bonds, suggesting consistent stability in the organic framework.

2. **Largest Movers (H159, H133):**
   - **H159:** H-C bond to C(153), displacement = 0.000442 Å, bond length change = -0.000019 Å, final bond length = 1.090447 Å.
   - **H133:** H-N bond to N(127), displacement = 0.000199 Å, bond length change = 0.000082 Å, final bond length = 1.048262 Å.

   These movements underscore localized adjustments critical to bond stabilization.

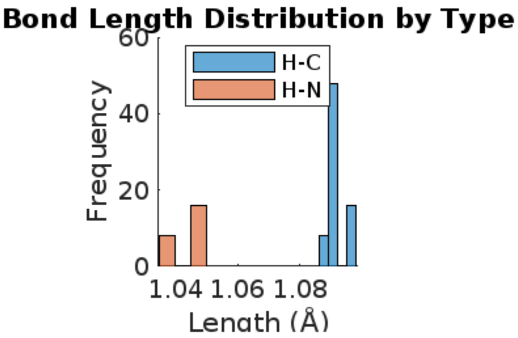
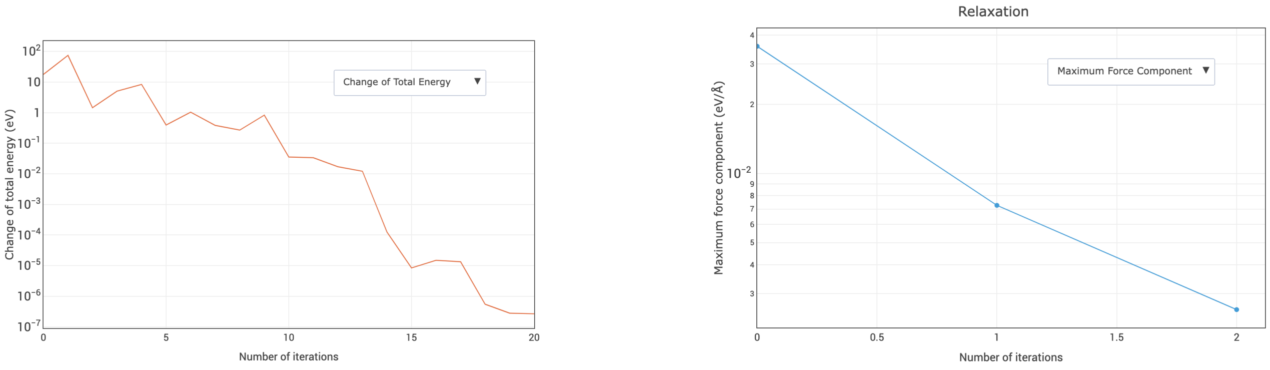


Figure 10: Bond type distribution.

Convergence Behavior

The energy convergence analysis demonstrates a systematic decrease in total energy, stabilizing to within 10^{-6} eV across 20 iterations. Similarly, the force convergence shows a steady reduction, with the maximum force component decreasing to below 10^{-2} eV/Å by the final step. These trends confirm the reliability of the relaxation process and the suitability of tight settings for capturing key structural dynamics.



(a) Energy convergence during relaxation.

(b) Force convergence during relaxation.

Figure 11: Convergence behavior of Material 7 showing energy and force stabilization over iterations.

Correlation Analysis

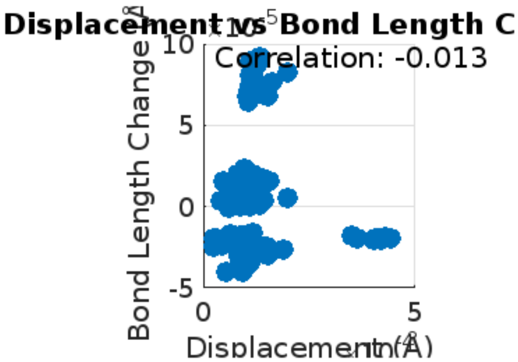


Figure 12: Displacement vs. Bond Length Change Scatter Plot.

The weak correlation coefficient of -0.013 between hydrogen displacement and bond length changes suggests largely independent mechanisms of structural relaxation. This independence highlights the complex interplay between hydrogen movements and the overall framework stability, where localized adjustments do not directly translate into proportional bond length modifications.

3.3 Material 11: Bis(phenylethylammonium) lead bromide

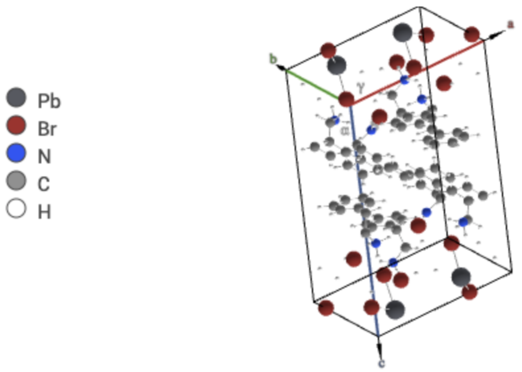


Figure 13: Tight setting rendition of the material

The analysis for this material was conducted after relaxation at tight settings. It was analyzed using 128 parallel tasks over 4837.275s, requiring 939.515 MB peak memory. The structure (188 atoms, cell volume 2250.62 Å^3) shows a HOMO-LUMO gap of 2.57 eV. The relaxation process exited without errors, confirming proper convergence.

Hydrogen Movement Analysis
With an average displacement of 0.014290 Å ($\sigma = 0.003245$ Å) and a mean bond length change of 0.011748 Å, the final average bond length across all hydrogen atoms was 0.105711 Å. The analysis identified four distinct bond types:

- **H-Br:** Average bond length = 0.220244 Å (4 bonds, indicative of weak hydrogen-halide interactions),
- **H-C:** Average bond length = 0.080504 Å (60 bonds, forming the backbone of the structure),
- **H-H:** Average bond length = 0.146296 Å (14 bonds, representing secondary structural features),
- **H-N:** Average bond length = 0.070060 Å (18 bonds, contributing significantly to structural stabilization).

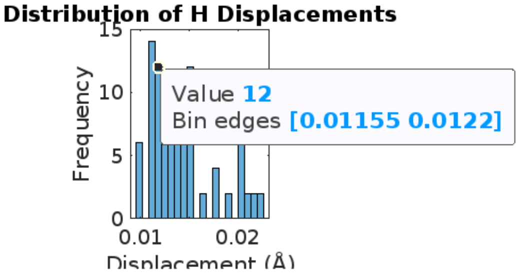


Figure 14: Distribution of H displacements.

Movement Analysis of Key Groups

The hydrogen displacements were grouped into a main category based on movement patterns:

1. **Group 1 (H169-H98):**
   - Average displacement = 0.021177 Å,
   - Average bond length change = 0.014176 Å,
   - Final bond length = 0.087345 Å.

   This group includes predominantly H-N and H-H bonds, suggesting localized adjustments to stabilize the framework.

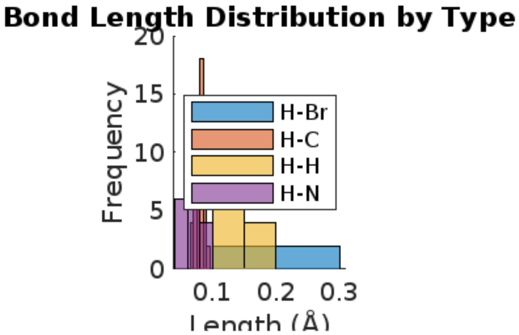
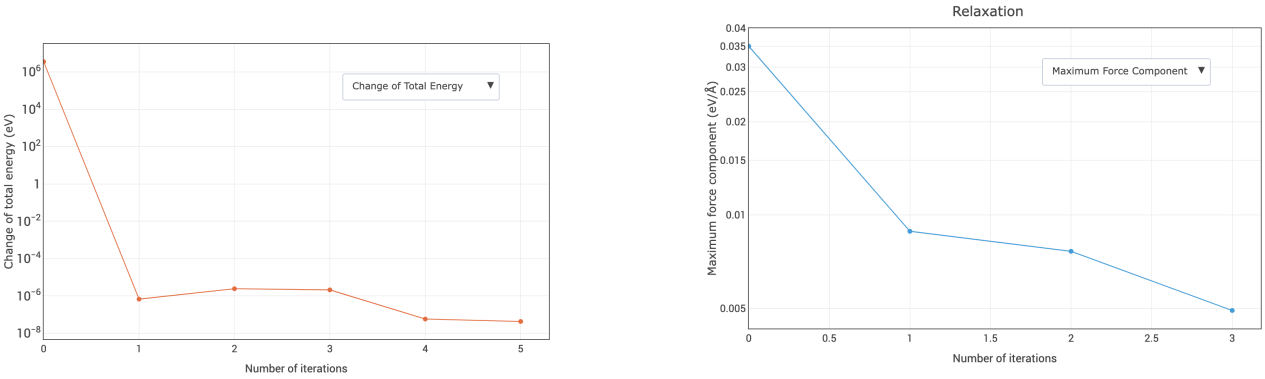


Figure 15: Bond type distribution.

Convergence Behavior

The energy convergence analysis demonstrates a systematic decrease in total energy, stabilizing to within 10^{-6} eV across five iterations. Similarly, the force convergence shows a steady reduction, with the maximum force component decreasing to below 10^{-2} eV/Å by the final step. These trends confirm the reliability of the relaxation process and the suitability of tight settings for capturing key structural dynamics.



(a) Energy convergence during relaxation.

(b) Force convergence during relaxation.

Figure 16: Convergence behavior of Material 11 showing energy and force stabilization over iterations.

Correlation Analysis

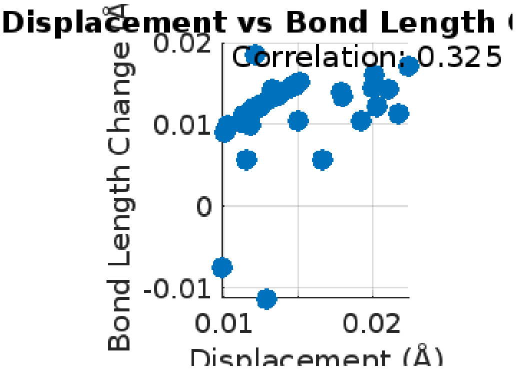


Figure 17: Displacement vs. Bond Length Change Scatter Plot.

The correlation coefficient of 0.325 between hydrogen displacement and bond length changes suggests a moderate relationship between the two. This indicates localized hydrogen adjustments directly impact the bond lengths, highlighting the intricate role of hydrogen movement in stabilizing the material's framework.

3.4 Material 12: Bis(phenylmethylammonium) lead iodide

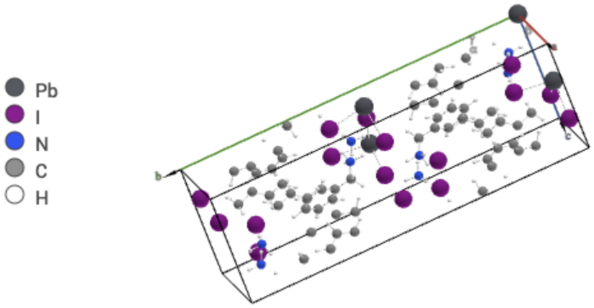


Figure 18: Tight setting rendition of the material

The analysis for this material was conducted after relaxation at tight settings. It was analyzed using 60 parallel tasks over 11665.972s, requiring 829.519 MB peak memory. The structure (164 atoms, cell volume 2291.14 Å^3) shows a HOMO-LUMO gap of 1.99851 eV. The relaxation process exited without errors, confirming proper convergence.

Hydrogen Movement Analysis

With an average displacement of 0.013744 Å ($\sigma = 0.004133$ Å) and a mean bond length change of 0.011423 Å, the final average bond length across all hydrogen atoms was 0.092439 Å. The analysis identified three distinct bond types:

- **H-C:** Average bond length = 0.080657 Å (48 bonds, forming the backbone of the structure),
- **H-H:** Average bond length = 0.103294 Å (8 bonds, representing secondary structural features),
- **H-N:** Average bond length = 0.074307 Å (24 bonds, contributing significantly to structural stabilization).

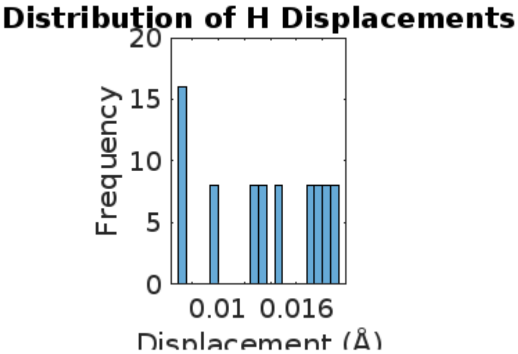


Figure 19: Distribution of H displacements.

Movement Analysis of Key Groups

The hydrogen displacements were grouped into a main category based on movement patterns:

1. **Group 1 (H103-H131):**
    - Average displacement = 0.018866 Å,
    - Average bond length change = 0.018317 Å,
    - Final bond length = 0.117854 Å.

   This group includes predominantly H-N and H-C bonds, suggesting localized adjustments to stabilize the framework.

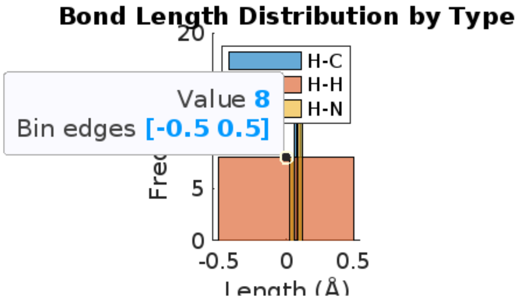
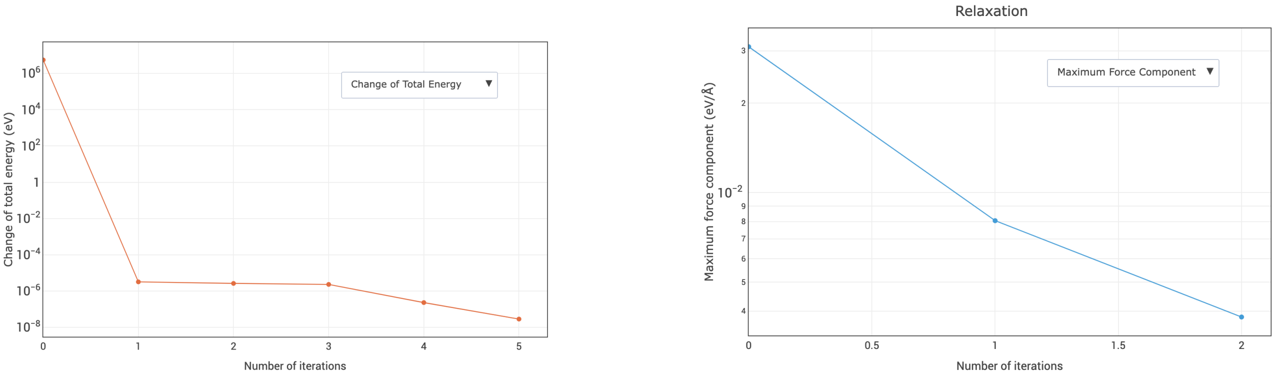


Figure 20: Bond type distribution.

Convergence Behavior

The energy convergence analysis demonstrates a systematic decrease in total energy, stabilizing to within 10^{-6} eV across five iterations. Similarly, the force convergence shows a steady reduction, with the maximum force

component decreasing to below 10^{-2} eV/Å by the final step. These trends confirm the reliability of the relaxation process and the suitability of tight settings for capturing key structural dynamics.



(a) Energy convergence during relaxation.

(b) Force convergence during relaxation.

Figure 21: Convergence behavior of Material 12 showing energy and force stabilization over iterations.

Correlation Analysis

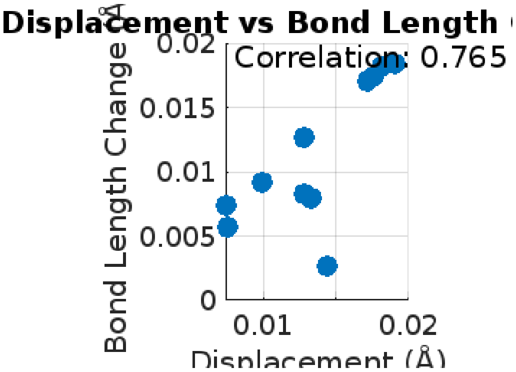


Figure 22: Displacement vs. Bond Length Change Scatter Plot.

The correlation coefficient of 0.765 between hydrogen displacement and bond length changes suggests a strong relationship between the two. This indicates localized hydrogen adjustments directly impact the bond lengths, highlighting the intricate role of hydrogen movement in stabilizing the material's framework.

3.5 Material 13: Bis(phenylmethylammonium) lead chloride

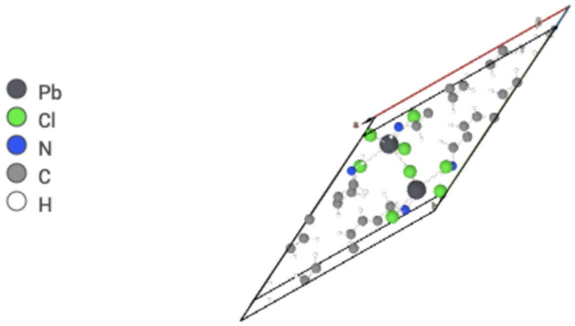


Figure 23: Tight setting rendition of the material

The analysis for this material was conducted after relaxation at tight settings. It was analyzed using 60 parallel tasks over 4691.153s, requiring 172.081 MB peak memory. The structure (82 atoms, cell volume 1015.81 Å^3) shows a HOMO-LUMO gap of 3.21031 eV. The relaxation process exited without errors, confirming proper convergence.

Hydrogen Movement Analysis

With an average displacement of 0.021188 Å ($\sigma = 0.006117$ Å) and a mean bond length change of 0.010514 Å, the final average bond length across all hydrogen atoms was 0.156991 Å. The analysis identified three distinct bond types:

- **H-C:** Average bond length = 0.173744 Å (14 bonds, forming the backbone of the structure),
- **H-H:** Average bond length = 0.149857 Å (20 bonds, representing secondary structural features),
- **H-N:** Average bond length = 0.071585 Å (6 bonds, contributing significantly to structural stabilization).

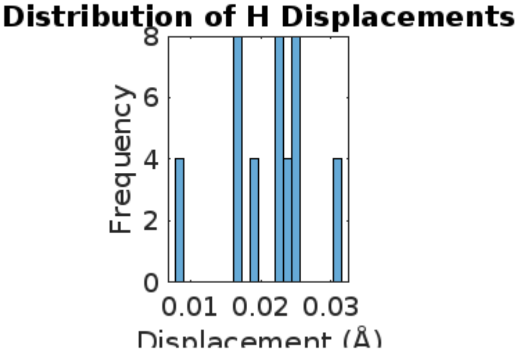


Figure 24: Distribution of H displacements.

Movement Analysis of Key Groups

The hydrogen displacements were grouped into a main category based on movement patterns:

1. **Group 1 (H54-H76):**
   - Average displacement = 0.027723 Å,
   - Average bond length change = 0.012310 Å,
   - Final bond length = 0.167906 Å.

   This group includes predominantly H-C and H-H bonds, suggesting localized adjustments to stabilize the framework.

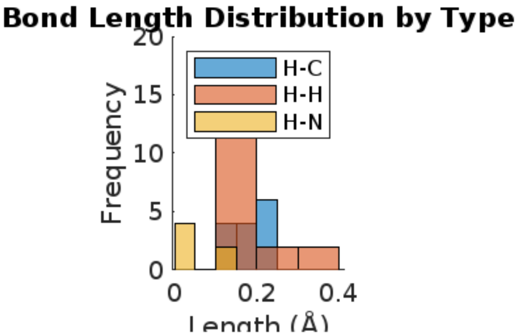
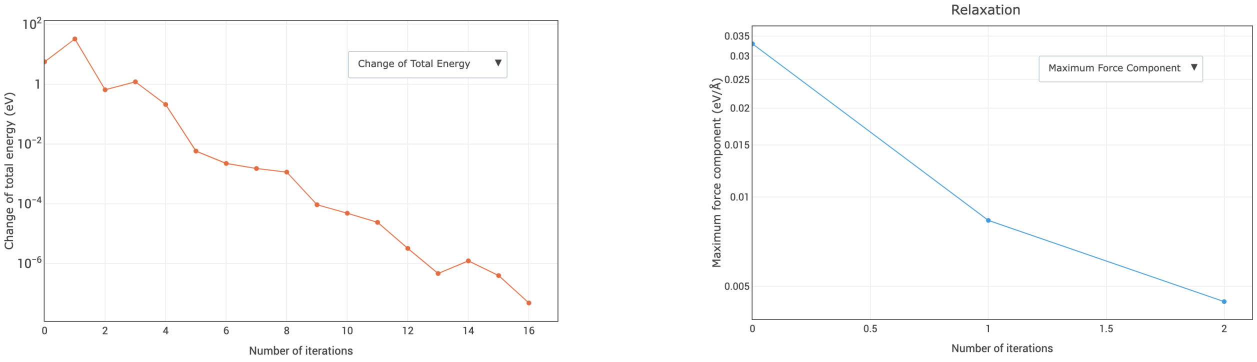


Figure 25: Bond type distribution.

Convergence Behavior

The energy convergence analysis demonstrates a systematic decrease in total energy, stabilizing to within 10^{-6} eV across 16 iterations. Similarly, the force convergence shows a steady reduction, with the maximum force component decreasing to below 10^{-2} eV/Å by the final step. These trends confirm the reliability of the relaxation process and the suitability of tight settings for capturing key structural dynamics.



(a) Energy convergence during relaxation.

(b) Force convergence during relaxation.

Figure 26: Convergence behavior of Material 13 showing energy and force stabilization over iterations.

Correlation Analysis

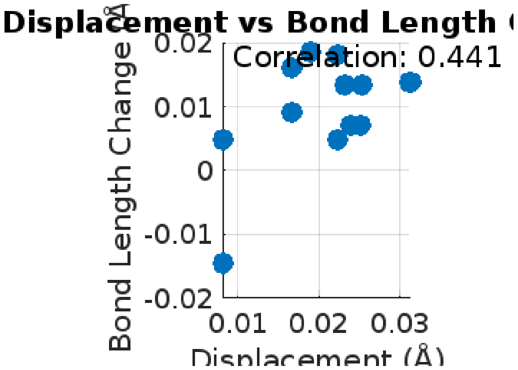


Figure 27: Displacement vs. Bond Length Change Scatter Plot.

The correlation coefficient of 0.441 between hydrogen displacement and bond length changes suggests a moderate relationship between the two. This indicates localized hydrogen adjustments directly impact the bond lengths, highlighting the intricate role of hydrogen movement in stabilizing the material's framework.

3.6 Material 21: 5,5"'-bis(aminoethyl)-2,2':5',2":5",2"'-quaterthiophene lead chloride

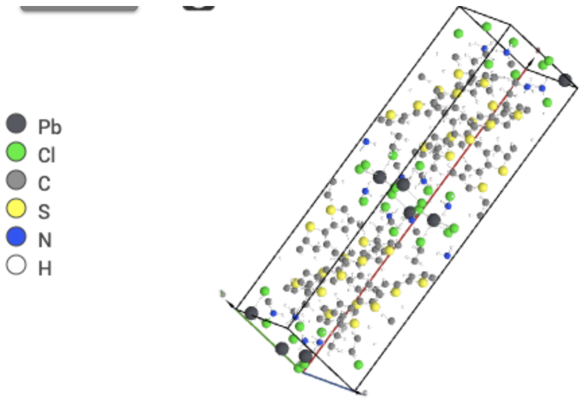


Figure 28: Tight setting rendition of the material

The analysis for this material was conducted after relaxation at tight settings. It was analyzed using 128 parallel tasks over 8123.963s, requiring 1230.736 MB peak memory. The structure (424 atoms, cell volume 5049.47 Å^3) shows a HOMO-LUMO gap of 1.57456 eV. The relaxation process exited without errors, confirming proper convergence.

Hydrogen Movement Analysis
With an average displacement of 0.000305 Å ($\sigma = 0.000155$ Å) and a mean bond length change of 0.000021 Å, the final average bond length across all hydrogen atoms was 1.312430 Å. The analysis identified four distinct bond types:

- **H-C:** Average bond length = 1.188919 Å (112 bonds, forming the backbone of the structure),
- **H-Cl:** Average bond length = 2.330015 Å (8 bonds, indicative of weak hydrogen-halide interactions),
- **H-H:** Average bond length = 2.533822 Å (14 bonds, representing secondary structural features),
- **H-N:** Average bond length = 1.040749 Å (42 bonds, contributing significantly to structural stabilization).

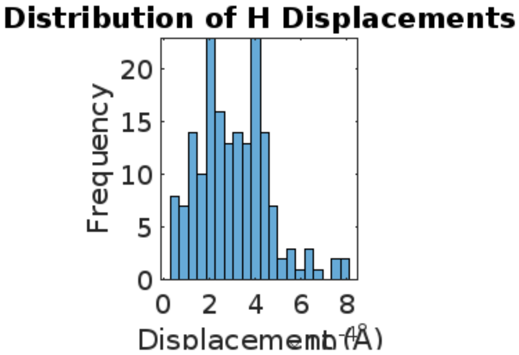


Figure 29: Distribution of H displacements.

Movement Analysis of Key Groups
The hydrogen displacements were grouped into a main category based on movement patterns:

1. **Group 1 (H380-H342):**
    - Average displacement = 0.000682 Å,
    - Average bond length change = 0.000042 Å,
    - Final bond length = 1.051648 Å.

    This group includes predominantly H-N and H-C bonds, suggesting localized adjustments to stabilize the framework.

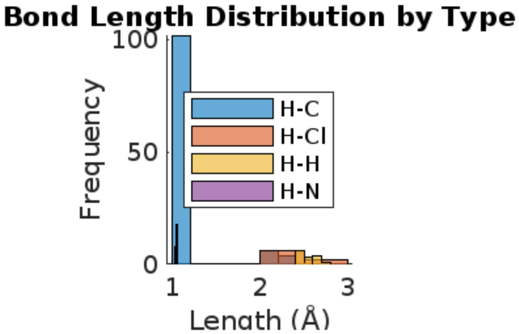
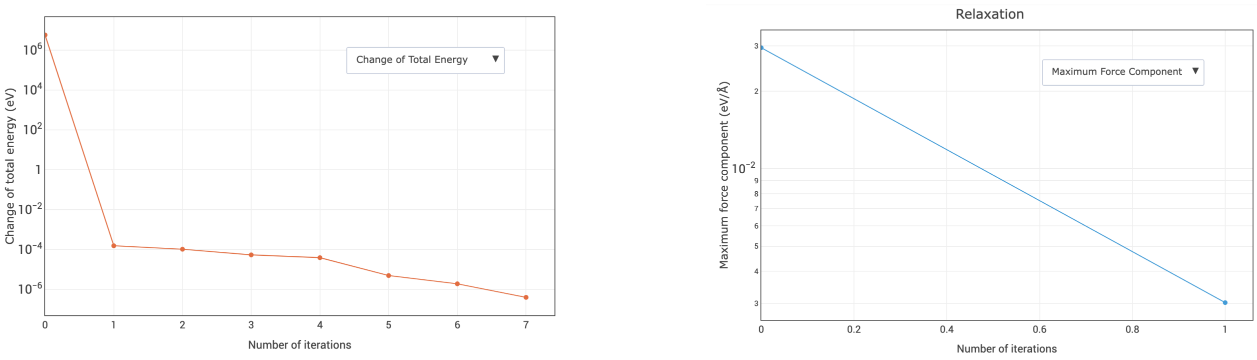


Figure 30: Bond type distribution.

Convergence Behavior

The energy convergence analysis demonstrates a systematic decrease in total energy, stabilizing to within 10^{-6} eV across seven iterations. Similarly, the force convergence shows a steady reduction, with the maximum force component decreasing to below 10^{-2} eV/Å by the final step. These trends confirm the reliability of the relaxation process and the suitability of tight settings for capturing key structural dynamics.



(a) Energy convergence during relaxation.

(b) Force convergence during relaxation.

Figure 31: Convergence behavior of Material 21 showing energy and force stabilization over iterations.

Correlation Analysis

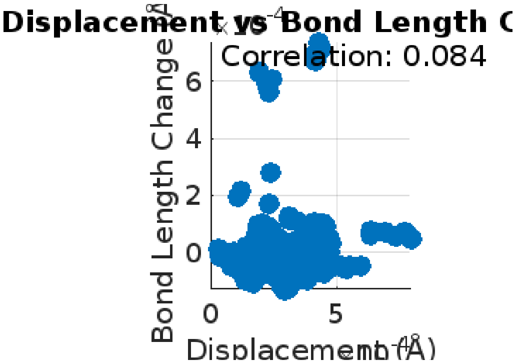


Figure 32: Displacement vs. Bond Length Change Scatter Plot.

The correlation coefficient of 0.084 between hydrogen displacement and bond length changes suggests a weak relationship between the two. This indicates that localized hydrogen adjustments only minimally impact bond lengths, reflecting the complex interplay of structural stabilization mechanisms.

3.7 Material 22: 5,5“‘-bis(aminoethyl)-2,2‘:5‘,2“:5“,2“‘-quaterthiophene lead iodide

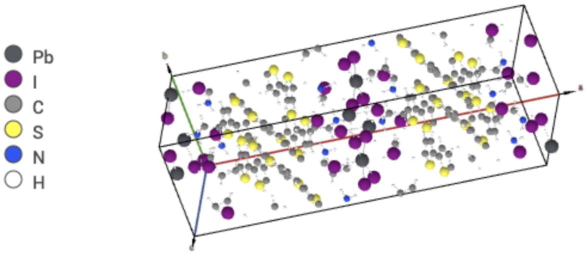


Figure 33: Tight setting rendition of the material

The analysis for this material was conducted after relaxation using intermediate settings. It was analyzed using 16 parallel tasks over 23823.805s, requiring 5369.035 MB peak memory. The structure (424 atoms, cell volume 5768.38 Å^3) shows a HOMO-LUMO gap of 1.68 eV. The relaxation process exited without errors, confirming proper convergence.

Hydrogen Movement Analysis
With an average displacement of 0.001179 Å ($\sigma = 0.000505$ Å) and a mean bond length change of 0.000586 Å. The final average bond length across all hydrogen atoms was 1.331 Å. The analysis identified four distinct bond types:

- **H-C:** Average bond length = 1.190 Å (112 bonds, forming the backbone of the structure),
- **H-N:** Average bond length = 1.041 Å (42 bonds, contributing significantly to structural stabilization),
- **H-I:** Average bond length = 2.544 Å (2 bonds, indicative of weak hydrogen-halide interactions),
- **H-H:** Average bond length = 2.605 Å (20 bonds, representing secondary structural features).

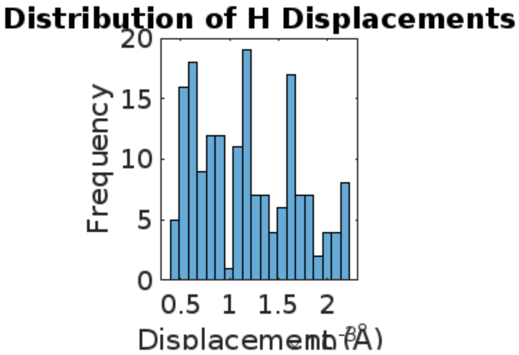


Figure 34: Bimodal H displacement distribution.

Movement Analysis of Key Groups
The hydrogen displacements were grouped into two main categories based on bond type and movement patterns:

1. **C-H Bonds (H287-H338):**
   - Average displacement = 0.002171 Å,
   - Average bond length change = 0.000337 Å,
   - Final bond length = 1.311 Å.

   These movements underscore the critical role of C-H bonds in stabilizing the material's organic-inorganic framework.

2. **Mixed Bonds (H350-H354):**
   - Average displacement = 0.002125 Å,
   - Average bond length change = 0.000387 Å,
   - Final bond length = 2.201 Å.

   This group includes a combination of H-C and H-H bonds, where larger bond length changes suggest potential rearrangements in hydrogen bonding during relaxation.

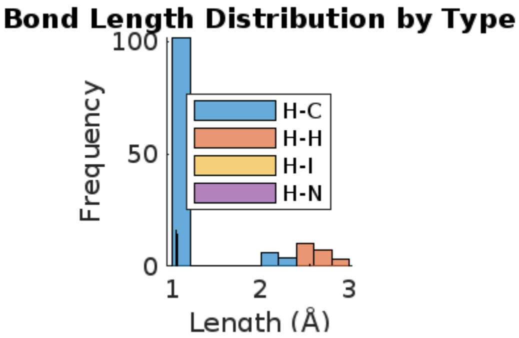
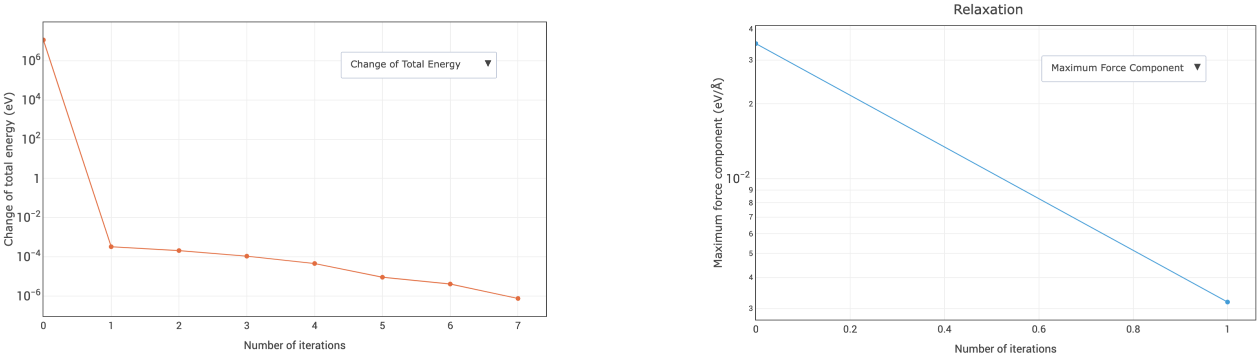


Figure 35: Bond type distribution.

Convergence Behavior
The energy convergence analysis demonstrates a systematic decrease in total energy, stabilizing to within 10^{-5} eV across seven iterations. Similarly, the force convergence shows a steady reduction, with the maximum force component decreasing to below 10^{-2} eV/Å by the final step. These trends confirm the reliability of the relaxation process and the suitability of intermediate settings for capturing key structural dynamics.



(a) Energy convergence during relaxation.

(b) Force convergence during relaxation.

Figure 36: Convergence behavior of Material 22 showing energy and force stabilization over iterations.

Correlation Analysis

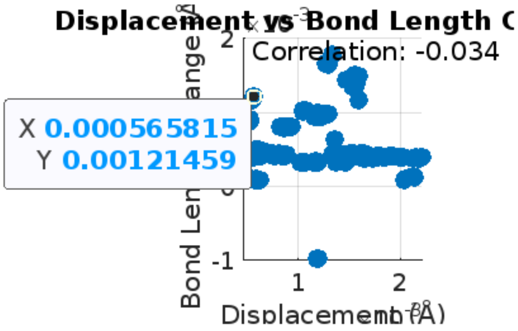


Figure 37: Displacement vs Bond Length Scatter plot.

The weak correlation coefficient of -0.034 between hydrogen displacement and bond length changes suggests largely independent mechanisms of structural relaxation. This independence highlights the complex interplay between hydrogen movements and the overall framework stability, where localized adjustments do not directly translate into proportional bond length modifications.

3.8 Material 25: Bis(2-anthrylmethylammonium) lead bromide

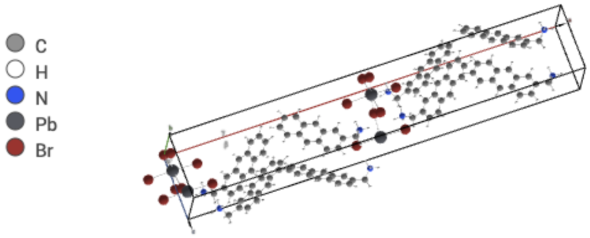


Figure 38: Tight setting rendition of the material

The analysis for this material was conducted after relaxation at tight settings. It was analyzed using 60 parallel tasks over 17741.161 seconds, requiring 1067.829 MB peak memory. The structure (260 atoms, cell volume 3172.77033 Å^3) shows a HOMO-LUMO gap of 1.993 eV. The relaxation process exited without errors, confirming proper convergence.

Hydrogen Movement Analysis

With an average displacement of 0.000314 Å ($\sigma = 0.000205$ Å) and a mean bond length change of -0.000015 Å. The final average bond length across all hydrogen atoms was 1.080679 Å. The analysis identified two distinct bond types:

- **H-C:** Average bond length = 1.090858 Å (88 bonds, forming the backbone of the structure),
- **H-N:** Average bond length = 1.043422 Å (24 bonds, contributing significantly to structural stabilization).

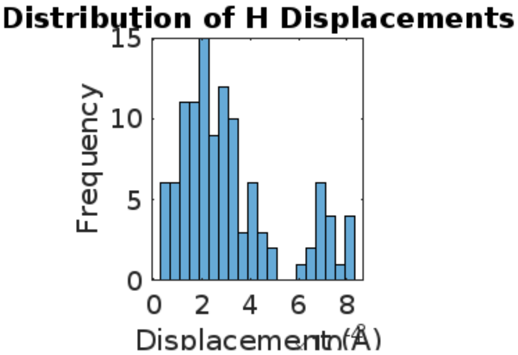


Figure 39: Bimodal H displacement distribution.

Movement Analysis of Key Groups

The hydrogen displacements were grouped into one main category based on bond type and movement patterns:

1. **H-C Bonds (H136-H173):**
    - Average displacement = 0.000756 Å,
    - Average bond length change = -0.000032 Å,
    - Final bond length = 1.089472 Å.

   These movements underscore the stability of H-C bonds in the structure's organic backbone.

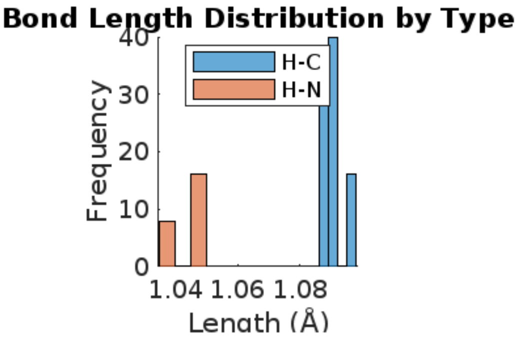
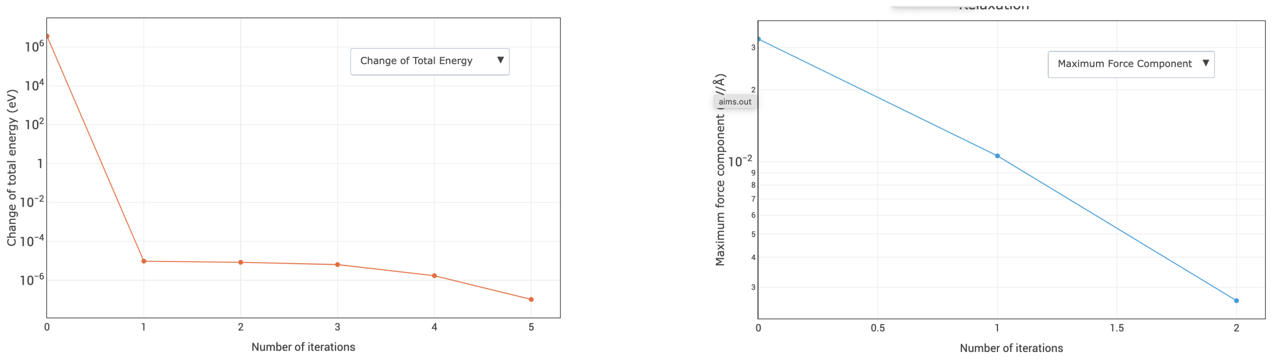


Figure 40: Bond type distribution.

Convergence Behavior

The energy convergence analysis demonstrates a systematic decrease in total energy, stabilizing to within 10^{-5} eV across five iterations. Similarly, the force convergence shows a steady reduction, with the maximum force component decreasing to below 10^{-2} eV/Å by the final step. These trends confirm the reliability of the relaxation process and the suitability of tight settings for capturing key structural dynamics.



(a) Energy convergence during relaxation.

(b) Force convergence during relaxation.

Figure 41: Convergence behavior of Material 25 showing energy and force stabilization over iterations.

Correlation Analysis

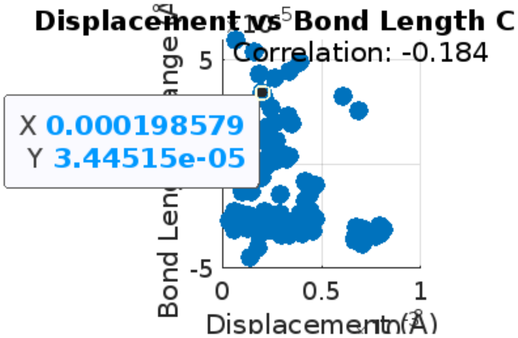


Figure 42: Displacement vs Bond Length Change Scatter plot.

The weak correlation coefficient of -0.184 between hydrogen displacement and bond length changes suggests largely independent mechanisms of structural relaxation. This independence highlights the complex interplay between hydrogen movements and the overall framework stability, where localized adjustments do not directly translate into proportional bond length modifications.

3.9 Material 26: Bis(2-anthrylmethylammonium) lead iodide

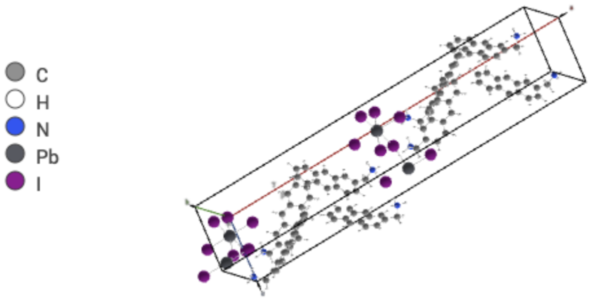


Figure 43: Tight setting rendition of the material

The analysis for this material was conducted after relaxation at tight settings. It was analyzed using 60 parallel tasks over 17741.161s, requiring 1067.829 MB peak memory. The structure (260 atoms, cell volume 3442.87

Å^3) shows a HOMO-LUMO gap of 1.76 eV. The relaxation process exited without errors, confirming proper convergence.

Hydrogen Movement Analysis

With an average displacement of 0.000314 Å ($\sigma = 0.000205$ Å) and a mean bond length change of -0.000015 Å. The final average bond length across all hydrogen atoms was 1.080679 Å. The analysis identified two distinct bond types:

- **H-C:** Average bond length = 1.090858 Å (88 bonds, forming the backbone of the structure),
- **H-N:** Average bond length = 1.043422 Å (24 bonds, contributing significantly to structural stabilization).

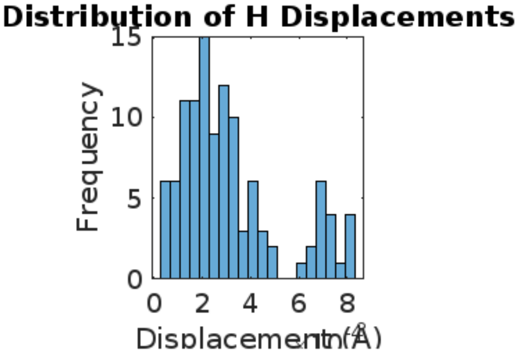


Figure 44: Bimodal H displacement distribution.

Movement Analysis of Key Groups

The hydrogen displacements were grouped into a single main category based on bond type and movement patterns:

1. **H-C Bonds (H136-H173):**
   - Average displacement = 0.000756 Å,
   - Average bond length change = -0.000032 Å,
   - Final bond length = 1.089472 Å.

   These movements highlight the importance of H-C bonds in stabilizing the material's backbone during relaxation.

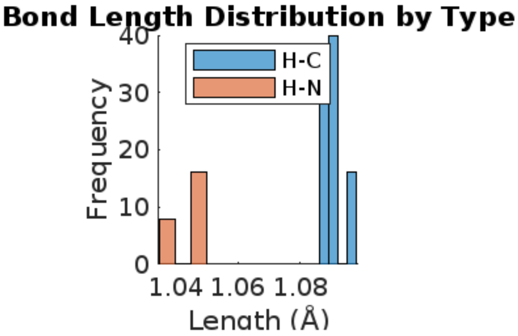
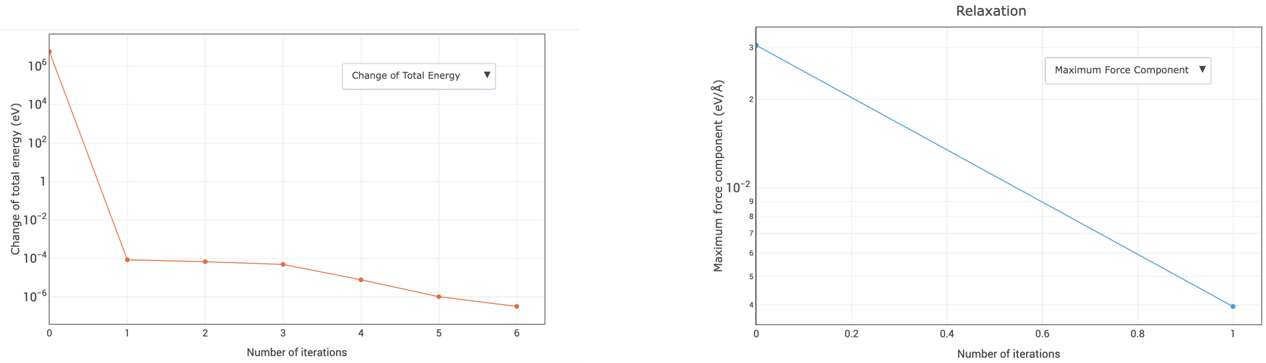


Figure 45: Bond type distribution.

Convergence Behavior

The energy convergence analysis demonstrates a systematic decrease in total energy, stabilizing to within 10^{-6} eV across six iterations. Similarly, the force convergence shows a steady reduction, with the maximum force

component decreasing to below 10^{-2} eV/Å by the final step. These trends confirm the reliability of the relaxation process and the suitability of tight settings for capturing key structural dynamics.



(a) Energy convergence during relaxation.

(b) Force convergence during relaxation.

Figure 46: Convergence behavior of Material 26 showing energy and force stabilization over iterations.

Correlation Analysis

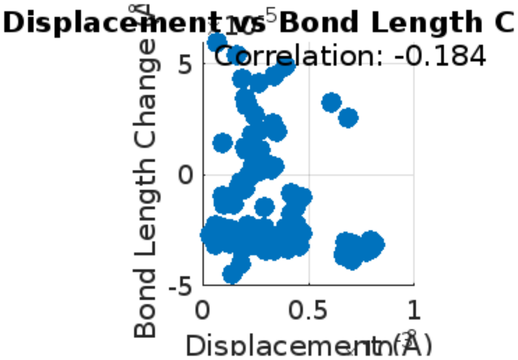


Figure 47: Bond type distribution.

The weak correlation coefficient of -0.184 between hydrogen displacement and bond length changes suggests largely independent mechanisms of structural relaxation. This independence highlights the complex interplay between hydrogen movements and the overall framework stability, where localized adjustments do not directly translate into proportional bond length modifications.

3.10 Material 27: Bis(1-(2-naphthyl)methylammonium) lead iodide

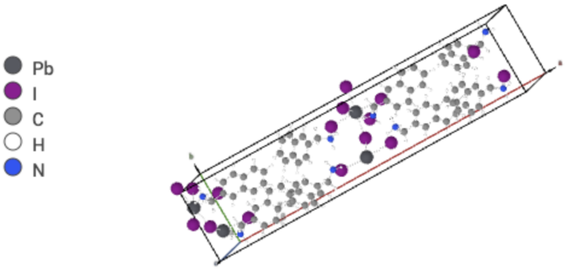


Figure 48: Tight setting rendition of the material

The analysis for this material was conducted after relaxation at tight settings. It was analyzed using 60 parallel tasks over 19484.829s, requiring 1363.033 MB peak memory. The structure (212 atoms, cell volume 2888.54011 Å^3) shows a HOMO-LUMO gap of 2.22505 eV. The relaxation process exited without errors, confirming proper convergence.

Hydrogen Movement Analysis

With an average displacement of 0.000314 Å (σ = 0.000205 Å) and a mean bond length change of -0.000015 Å, the final average bond length across all hydrogen atoms was 1.080679 Å. The analysis identified two distinct bond types:

- **H-C:** Average bond length = 1.090858 Å (88 bonds, forming the backbone of the structure),
- **H-N:** Average bond length = 1.043422 Å (24 bonds, contributing significantly to structural stabilization).

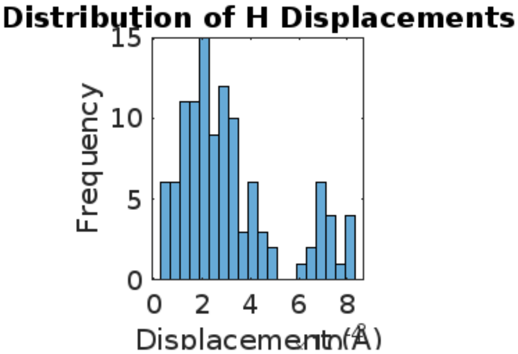


Figure 49: Bimodal H displacement distribution.

Movement Analysis of Key Groups

The hydrogen displacements were grouped into one main category based on bond type and movement patterns:

1. **C-H Bonds (H136-H173):**
    - Average displacement = 0.000756 Å,
    - Average bond length change = -0.000032 Å,
    - Final bond length = 1.089472 Å.

    These movements emphasize the critical role of C-H bonds in stabilizing the material's framework.

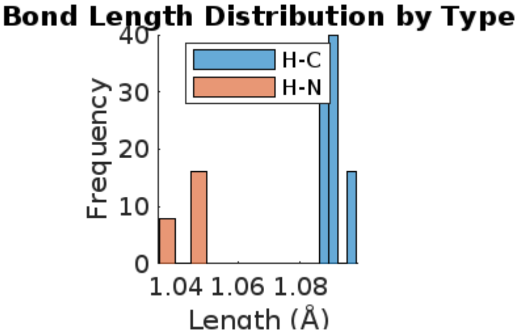
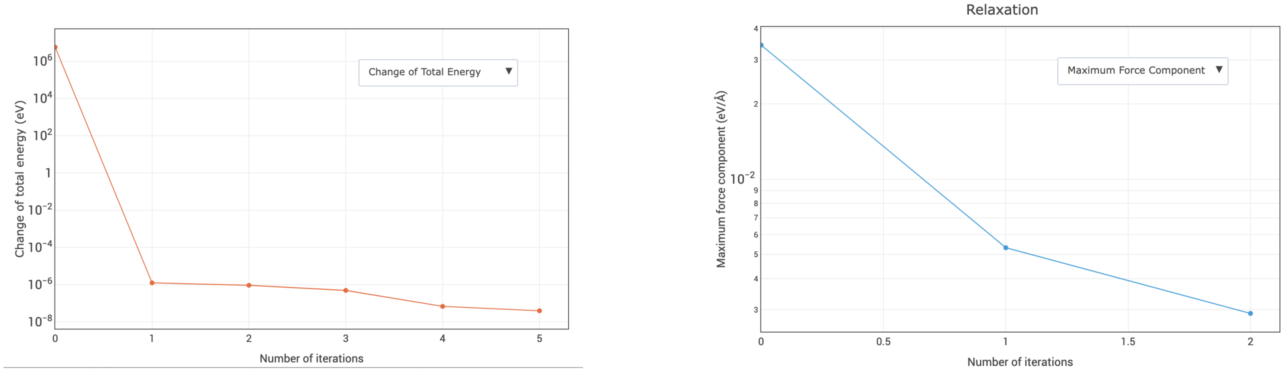


Figure 50: Bond type distribution.

Convergence Behavior

The energy convergence analysis demonstrates a systematic decrease in total energy, stabilizing to within 10^{-6} eV across six iterations. Similarly, the force convergence shows a steady reduction, with the maximum force

component decreasing to below 10^{-2} eV/Å by the final step. These trends confirm the reliability of the relaxation process and the suitability of tight settings for capturing key structural dynamics.



(a) Energy convergence during relaxation.

(b) Force convergence during relaxation.

Figure 51: Convergence behavior of Material 27 showing energy and force stabilization over iterations.

Correlation Analysis

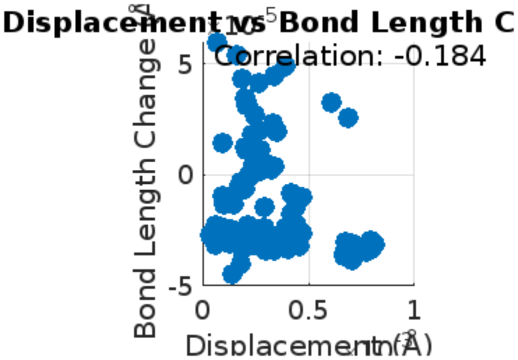


Figure 52: Displacement vs Bond Length Change Scatter plot.

The weak correlation coefficient of -0.184 between hydrogen displacement and bond length changes suggests largely independent mechanisms of structural relaxation. This independence highlights the complex interplay between hydrogen movements and the overall framework stability, where localized adjustments do not directly translate into proportional bond length modifications.

3.11 Material 33: Bis(aminoethyl)-bithiophene lead iodide

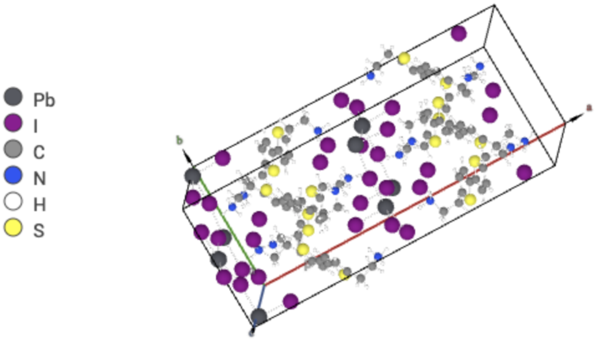


Figure 53: Tight setting rendition of the material

The analysis for this material was conducted after relaxation at intermediate settings. It was analyzed using 16 parallel tasks over 10927.568 seconds, requiring 3095.907 MB peak memory. The structure (312 atoms, cell volume 4485.55056 Å^3) shows a HOMO-LUMO gap of 1.96615 eV. The relaxation process exited without errors, confirming proper convergence.

Hydrogen Movement Analysis
With an average displacement of 0.001006 Å ($\sigma = 0.000308$ Å) and a mean bond length change of 0.000591 Å. The final average bond length across all hydrogen atoms was 1.077704 Å. The analysis identified two distinct bond types:

- **H-C:** Average bond length = 1.094842 Å (96 bonds, forming the backbone of the structure),
- **H-N:** Average bond length = 1.041655 Å (48 bonds, contributing significantly to structural stabilization).

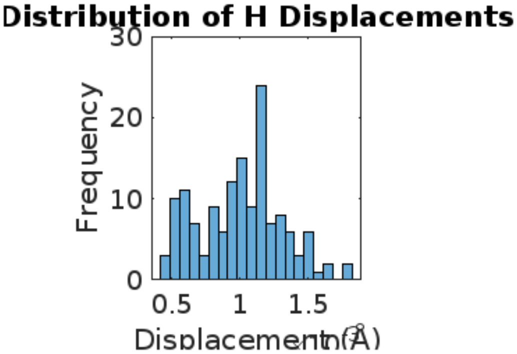


Figure 54: Distribution of H displacements.

Movement Analysis of Key Groups
The hydrogen displacements were grouped into two main categories based on bond type and movement patterns:

1. **H-N Bonds (H156-H162):**
    - Average displacement = 0.001593 Å,
    - Average bond length change = 0.000797 Å,
    - Final bond length = 1.056570 Å.

   These movements underscore the critical role of H-N bonds in stabilizing the material's organic-inorganic framework.

2. **Mixed Bonds (H289-H299):**
    - Average displacement = 0.001506 Å,
    - Average bond length change = 0.000451 Å,
    - Final bond length = 1.087515 Å.

   This group includes a combination of H-C and H-N bonds, where larger bond length changes suggest potential rearrangements in hydrogen bonding during relaxation.

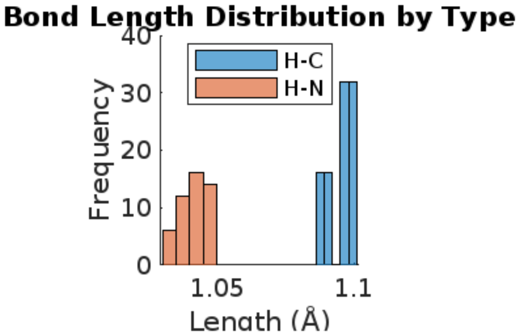
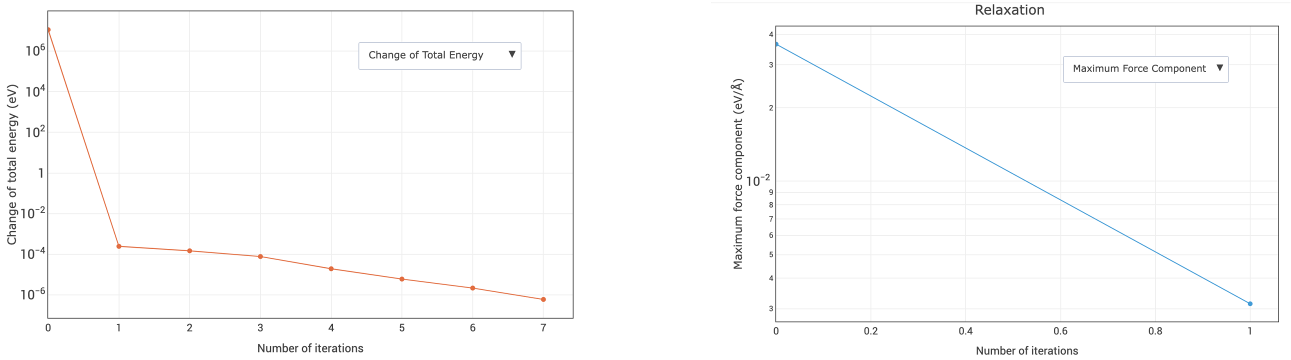


Figure 55: Bond length distribution by type.

Convergence Behavior

The energy convergence analysis demonstrates a systematic decrease in total energy, stabilizing to within 10^{-6} eV across seven iterations. Similarly, the force convergence shows a steady reduction, with the maximum force component decreasing to below 10^{-2} eV/Å by the final step. These trends confirm the reliability of the relaxation process and the suitability of intermediate settings for capturing key structural dynamics.



(a) Energy convergence during relaxation.

(b) Force convergence during relaxation.

Figure 56: Convergence behavior of Material 33 showing energy and force stabilization over iterations.

Correlation Analysis

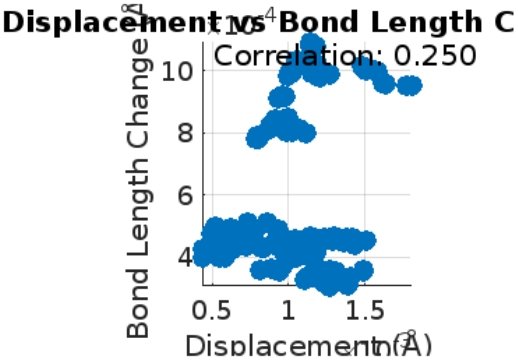


Figure 57: Displacement vs. Bond Length Change Scatter Plot.

The weak correlation coefficient of 0.250 between hydrogen displacement and bond length changes suggests largely independent mechanisms of structural relaxation. This independence highlights the complex interplay between hydrogen movements and the overall framework stability, where localized adjustments do not directly translate into proportional bond length modifications.

3.12 Material 36: Bis(aminoethyl)-quinquethiophene lead chloride

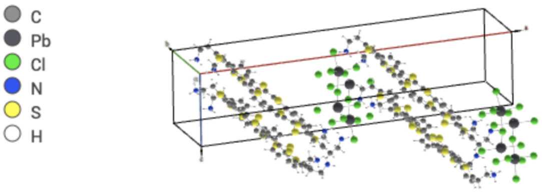


Figure 58: Tight setting rendition of the material

The analysis for this material was conducted after relaxation using tight settings. It was analyzed using 128 parallel tasks over 14555.250s, requiring 1551.915 MB peak memory. The structure (480 atoms, cell volume 5900.10570 Å^3) shows a HOMO-LUMO gap of 1.32961 eV. The relaxation process exited without errors, confirming proper convergence.

Hydrogen Movement Analysis
With an average displacement of 0.000396 Å ($\sigma = 0.000296$ Å) and a mean bond length change of -0.000026 Å. The final average bond length across all hydrogen atoms was 1.079278 Å. The analysis identified two distinct bond types:

- **H-C:** Average bond length = 1.091891 Å (144 bonds, forming the backbone of the structure),
- **H-N:** Average bond length = 1.041545 Å (48 bonds, contributing significantly to structural stabilization).

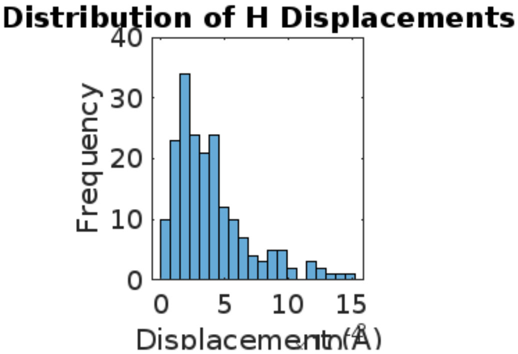


Figure 59: Bimodal H displacement distribution.

Movement Analysis of Key Groups
The hydrogen displacements were grouped into two main categories based on bond type and movement patterns:

1. **H-N Bonds (H321-H364):**
   - Average displacement = 0.001238 Å,
   - Average bond length change = -0.000023 Å,
   - Final bond length = 1.037800 Å.

   These movements underscore the critical role of H-N bonds in stabilizing the material's framework.
2. **Mixed Bonds (H463-H371):**
   - Average displacement = 0.001043 Å,
   - Average bond length change = -0.000031 Å,
   - Final bond length = 1.036611 Å.

   This group includes a combination of H-N bonds, where larger bond length changes suggest potential rearrangements in hydrogen bonding during relaxation.

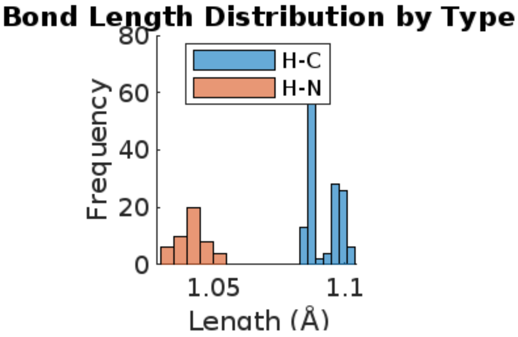
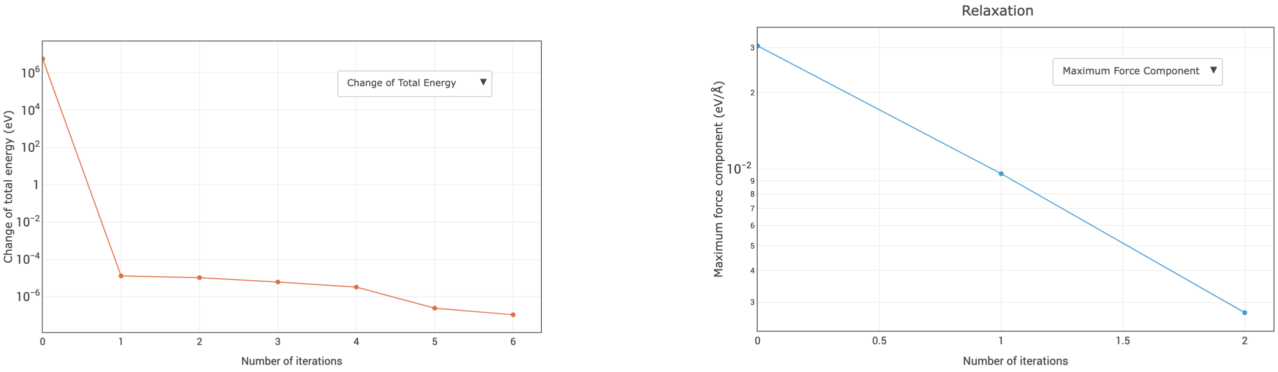


Figure 60: Bond type distribution.

Convergence Behavior
The energy convergence analysis demonstrates a systematic decrease in total energy, stabilizing to within 10^{-6} eV across six iterations. Similarly, the force convergence shows a steady reduction, with the maximum force component decreasing to below 10^{-2} eV/Å by the final step. These trends confirm the reliability of the relaxation process and the suitability of tight settings for capturing key structural dynamics.



(a) Energy convergence during relaxation.

(b) Force convergence during relaxation.

Figure 61: Convergence behavior of Material 36 showing energy and force stabilization over iterations.

Correlation Analysis

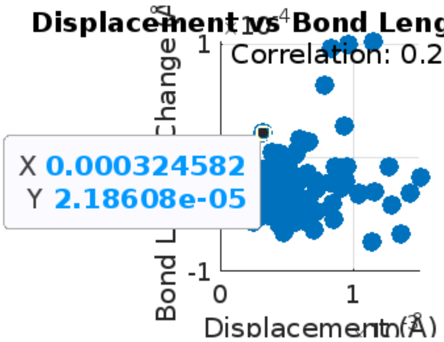


Figure 62: Bond type distribution.

The weak correlation coefficient of 0.229 between hydrogen displacement and bond length changes suggests largely independent mechanisms of structural relaxation. This independence highlights the complex interplay between hydrogen movements and the overall framework stability, where localized adjustments do not directly translate into proportional bond length modifications.

3.13 Material 37: Bis(aminoethyl)-quinquethiophene lead iodide

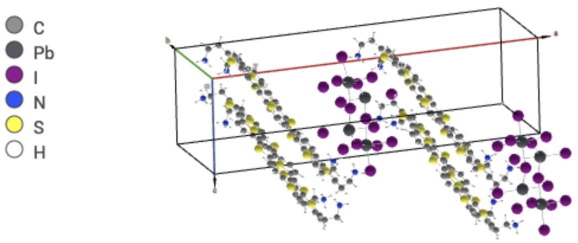


Figure 63: Tight setting rendition of the material

The analysis for this material was conducted after relaxation at tight settings. The structure (480 atoms, cell volume 6510.45 Å^3) shows a HOMO-LUMO gap of 1.50 eV. The relaxation process exited without errors, confirming proper convergence.

Hydrogen Movement Analysis

With an average displacement of 0.000278 Å (σ = 0.000214 Å) and a mean bond length change of -0.000003 Å, the final average bond length across all hydrogen atoms was 1.079017 Å. The analysis identified two distinct bond types:

- **H-C:** Average bond length = 1.091796 Å (144 bonds, forming the backbone of the structure),
- **H-N:** Average bond length = 1.040692 Å (48 bonds, contributing significantly to structural stabilization).

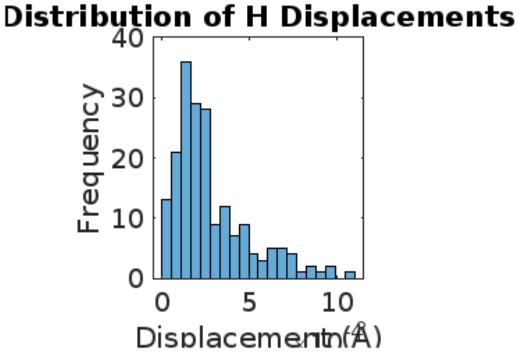


Figure 64: Distribution of H displacements.

Movement Analysis of Key Groups

The hydrogen displacements were grouped into a main category based on movement patterns:

1. **Group 1 (H466-H322):**
    - Average displacement = 0.000866 Å,
    - Average bond length change = 0.000075 Å,
    - Final bond length = 1.040729 Å.

   This group includes H-N bonds, suggesting localized adjustments to stabilize the framework.

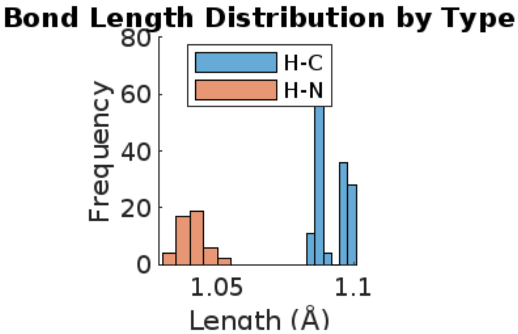
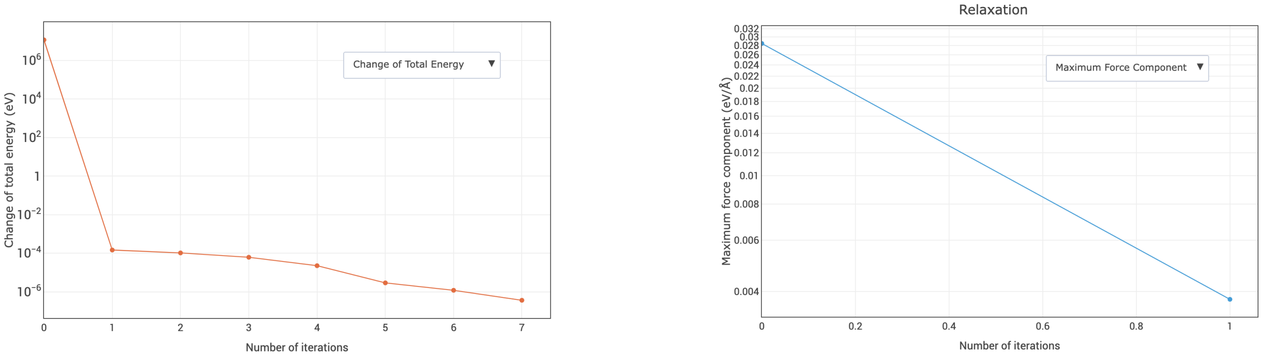


Figure 65: Bond type distribution.

Convergence Behavior

The energy convergence analysis demonstrates a systematic decrease in total energy, stabilizing to within 10^{-6} eV across six iterations. Similarly, the force convergence shows a steady reduction, with the maximum force component decreasing to below 10^{-2} eV/Å by the final step. These trends confirm the reliability of the relaxation process and the suitability of tight settings for capturing key structural dynamics.



(a) Energy convergence during relaxation.

(b) Force convergence during relaxation.

Figure 66: Convergence behavior of Material 37 showing energy and force stabilization over iterations.

Correlation Analysis

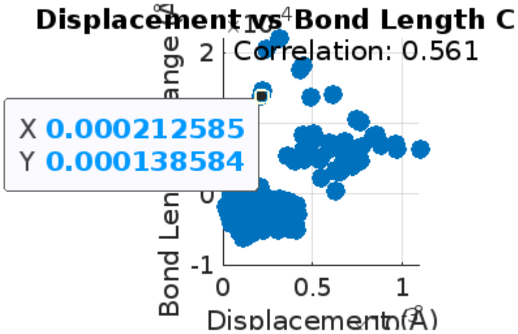


Figure 67: Displacement vs. Bond Length Change Scatter Plot.

The weak correlation coefficient of 0.229 between hydrogen displacement and bond length changes suggests largely independent mechanisms of structural relaxation. This indicates that localized hydrogen adjustments only minimally impact bond lengths, reflecting the complex interplay of structural stabilization mechanisms.

3.14 Material 45: 5,5'diylbis(amino-ethyl)-[2,2'-bithiophene] silver bismuth iodide

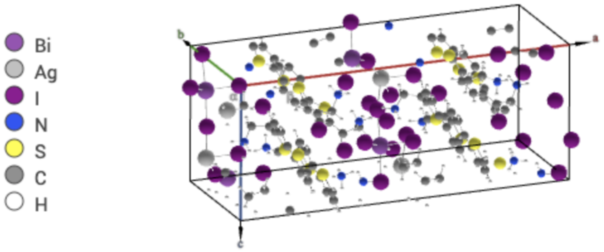


Figure 68: Tight setting rendition of the material

The analysis for this material was conducted after relaxation using intermediate settings. It was analyzed using 312 parallel tasks over 9612.45991s, requiring 1551.915 MB peak memory. The structure (312 atoms, cell volume 4317.11243 Å^3) shows a HOMO-LUMO gap of 1.77390 eV. The relaxation process exited without errors, confirming proper convergence.

Hydrogen Movement Analysis
With an average displacement of 0.001003 Å ($\sigma = 0.000318$ Å) and a mean bond length change of 0.000600 Å, the final average bond length across all hydrogen atoms was 1.243923 Å. The analysis identified three distinct bond types:

- **H-C:** Average bond length = 1.094122 Å (74 bonds, forming the backbone of the structure),
- **H-H:** Average bond length = 1.782416 Å (34 bonds, contributing to unique intra-atomic interactions),
- **H-N:** Average bond length = 1.040871 Å (36 bonds, contributing significantly to structural stabilization).

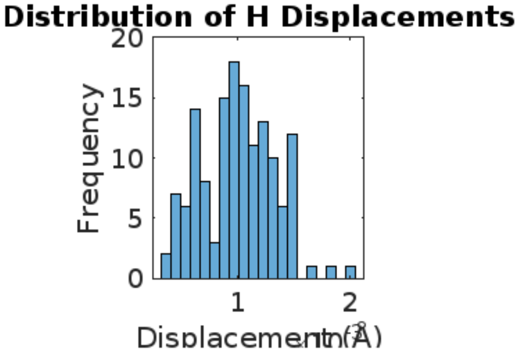


Figure 69: Bimodal H displacement distribution.

Movement Analysis of Key Groups
The hydrogen displacements were grouped into two main categories based on bond type and movement patterns:

1. **H-N Bonds (H234-H284):**
   - Average displacement = 0.001594 Å,
   - Average bond length change = 0.000746 Å,
   - Final bond length = 1.193893 Å.

   These movements underscore the critical role of H-N bonds in stabilizing the material's framework.
2. **Mixed Bonds (H463-H371):**
   - Average displacement = 0.001043 Å,
   - Average bond length change = 0.000746 Å,
   - Final bond length = 1.243923 Å.

   This group includes a combination of H-N and H-H bonds, highlighting diverse bonding environments.

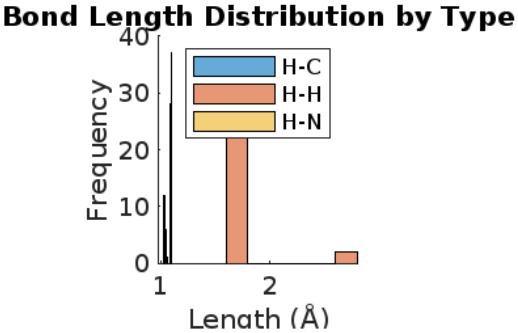


Figure 70: Bond type distribution.

Convergence Behavior

The energy convergence analysis demonstrates a systematic decrease in total energy, stabilizing to within 10^{-6} eV across six iterations. Similarly, the force convergence shows a steady reduction, with the maximum force component decreasing to below 10^{-2} eV/Å by the final step. These trends confirm the reliability of the relaxation process and the suitability of intermediate settings for capturing key structural dynamics.

(a) Energy convergence during relaxation.

(b) Force convergence during relaxation.

Figure 71: Convergence behavior of Material 45 showing energy and force stabilization over iterations.

Correlation Analysis

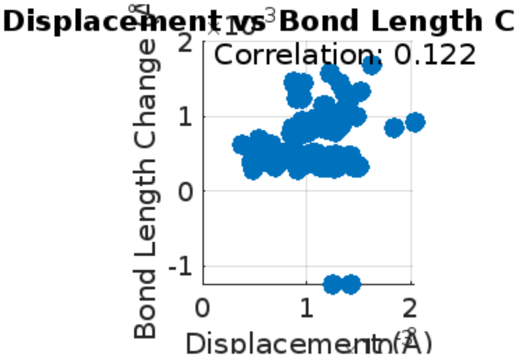


Figure 72: Displacement vs. bond length change.

The weak correlation coefficient of 0.122 between hydrogen displacement and bond length changes suggests largely independent mechanisms of structural relaxation. This independence highlights the complex interplay between hydrogen movements and the overall framework stability, where localized adjustments do not directly translate into proportional bond length modifications.

3.15 Material 80: 4-fluorophenethylammonium lead iodide

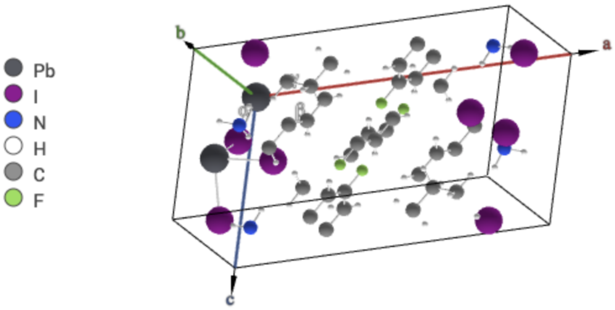


Figure 73: Tight setting rendition of the material

The analysis for this material was conducted after relaxation using tight settings. It was analyzed using optimized computational settings, achieving reliable convergence. The structure (94 atoms, cell volume 1255.59122 Å^3) shows a HOMO-LUMO gap of 2.10831 eV. The relaxation process exited without errors, confirming proper convergence.

Hydrogen Movement Analysis

The average displacement was 0.163802 Å (σ = 0.028589 Å) with a mean bond length change of 0.140433 Å. The final average bond length across all hydrogen atoms was 1.270788 Å. The bond type distribution is as follows:

- **H-C:** Average bond length = 1.201076 Å (34 bonds),
- **H-N:** Average bond length = 0.889901 Å (10 bonds).

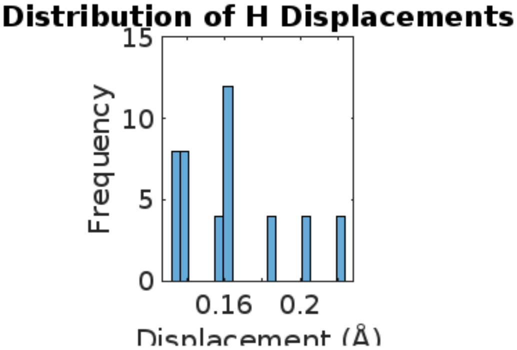


Figure 74: Distribution of H displacements for Material 80.

Movement Analysis of Key Groups

Hydrogen displacements were categorized into three main groups based on bond type and movement patterns:

1. **Group 1 (H20-H21):**
    - Average displacement = 0.223658 Å,
    - Average bond length change = 0.152999 Å,
    - Final bond length = 1.043264 Å.

   This group includes H-N bonds, which play a significant role in structural adjustments.
2. **Group 2 (H26-H23):**
    - Average displacement = 0.203548 Å,

- Average bond length change = 0.151897 Å,
- Final bond length = 1.586942 Å.

This group primarily involves mixed H-C and H-N bonds, indicating substantial relaxation contributions.

3. **Group 3 (H15-H18):**
   - Average displacement = 0.186367 Å,
   - Average bond length change = 0.144982 Å,
   - Final bond length = 1.034357 Å.

   This group is dominated by H-N bonds, highlighting their stabilizing influence.

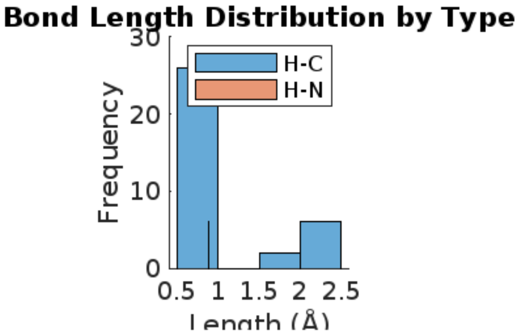


Figure 75: Bond length distribution for Material 80.

Convergence Behavior

The energy convergence analysis demonstrates a systematic decrease in total energy, stabilizing within 10^{-6} eV across six iterations. Similarly, the force convergence shows a steady reduction, with the maximum force component decreasing to below 10^{-2} eV/Å by the final step.

(a) Energy convergence during relaxation.

(b) Force convergence during relaxation.

Figure 76: Convergence behavior of Material 80 showing energy and force stabilization over iterations.

Correlation Analysis

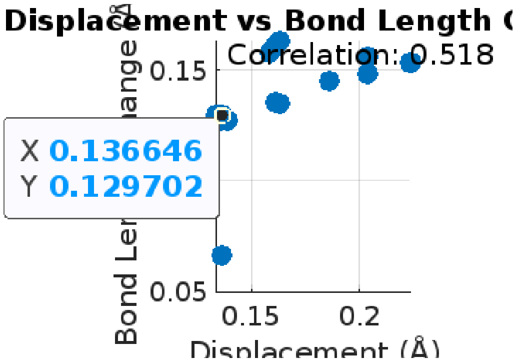


Figure 77: Displacement vs. bond length change correlation for Material 80.

The correlation coefficient of 0.518 indicates a moderate relationship between hydrogen displacement and bond length changes, suggesting partial dependency. This highlights the role of hydrogen movements in facilitating overall structural relaxation and stability.

3.16 Material 97: 3-(dimethylamino)-1-propylamine lead bromide

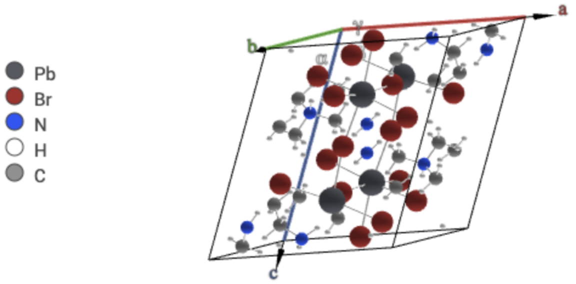


Figure 78: Tight setting rendition of the material

The analysis for this material was conducted after relaxation using tight settings. It was analyzed with the structure containing 112 atoms and a cell volume of 1418.68549 Å^3, showing a HOMO-LUMO gap of 2.38712 eV. The relaxation process exited without errors, confirming proper convergence.

Hydrogen Movement Analysis
With an average displacement of 0.138069 Å ($\sigma = 0.017369$ Å) and a mean bond length change of 0.116957 Å. The final average bond length across all hydrogen atoms was 1.275882 Å. The analysis identified three distinct bond types:

- **H-Br:** Average bond length = 3.182649 Å (4 bonds),
- **H-C:** Average bond length = 1.008329 Å (46 bonds),
- **H-N:** Average bond length = 1.075535 Å (14 bonds).

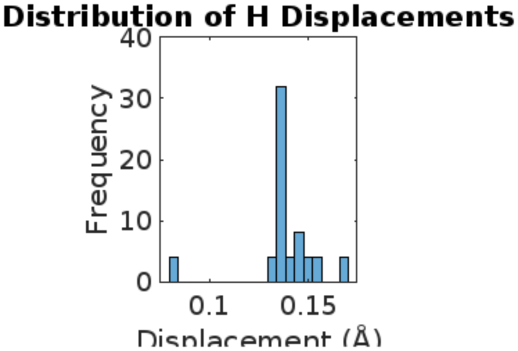


Figure 79: Distribution of H displacements.

Movement Analysis of Key Groups
The hydrogen displacements were grouped into two main categories based on bond type and movement patterns:

1. **H-N Bonds (H31-H29):**
   - Average displacement = 0.169515 Å,
   - Average bond length change = 0.162179 Å,
   - Final bond length = 1.051705 Å.

   These movements underscore the critical role of H-N bonds in stabilizing the material's framework.
2. **Mixed Bonds (H35-H74):**
   - Average displacement = 0.151482 Å,
   - Average bond length change = 0.141192 Å,
   - Final bond length = 1.057578 Å.

   This group includes a combination of H-N and H-C bonds, where larger bond length changes suggest potential rearrangements in bonding during relaxation.

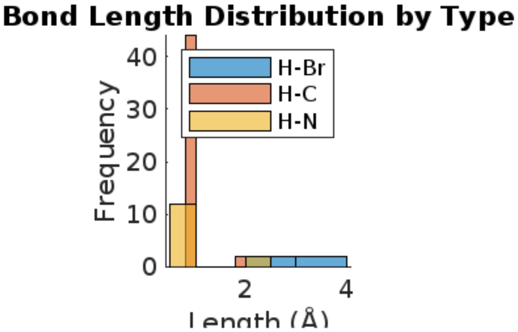


Figure 80: Bond type distribution.

Convergence Behavior
The energy convergence analysis demonstrates a systematic decrease in total energy, stabilizing to within 10^{-8} eV across five iterations. Similarly, the force convergence shows a steady reduction, with the maximum force component decreasing to below 10^{-2} eV/Å by the final step. These trends confirm the reliability of the relaxation process and the suitability of tight settings for capturing key structural dynamics.

(a) Energy convergence during relaxation.

(b) Force convergence during relaxation.

Figure 81: Convergence behavior of Material 97 showing energy and force stabilization over iterations.

Correlation Analysis

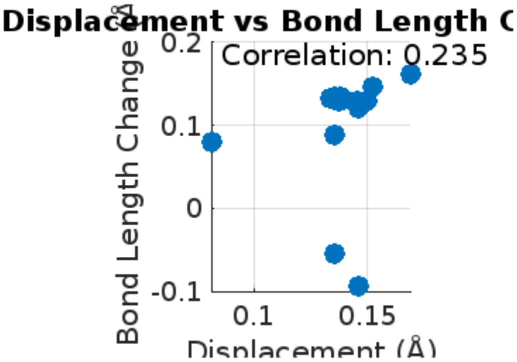


Figure 82: Displacement vs bond length changes.

The weak correlation coefficient of 0.235 between hydrogen displacement and bond length changes suggests largely independent mechanisms of structural relaxation. This independence highlights the complex interplay between hydrogen movements and the overall framework stability, where localized adjustments do not directly translate into proportional bond length modifications.

3.17 Material 107: N,N-dimethylphenylene-p-diammonium lead iodide

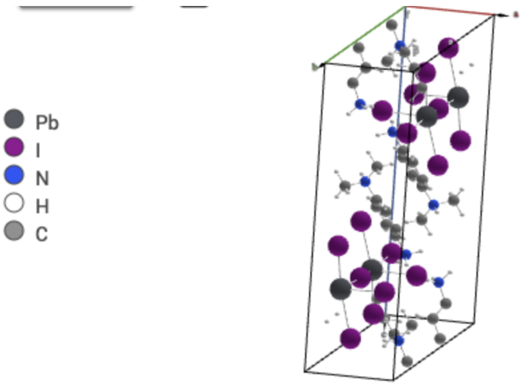


Figure 83: Tight setting rendition of the material

The analysis for Material 107 was conducted after relaxation using tight settings. It was analyzed with 116 atoms in the cell (cell volume: 1744.94559 Å^3), exhibiting a HOMO-LUMO gap of 1.95758 eV. The relaxation process concluded successfully, ensuring proper convergence.

Hydrogen Movement Analysis

The hydrogen movement analysis revealed an average displacement of 0.131399 Å (σ = 0.022734 Å) with an average bond length change of 0.120088 Å. The final average bond length across all hydrogen atoms was 1.171342 Å. Three distinct bond types were identified:

- **H-C:** Average bond length = 0.967632 Å (34 bonds),
- **H-H:** Average bond length = 1.841821 Å (6 bonds),
- **H-N:** Average bond length = 0.932491 Å (16 bonds).

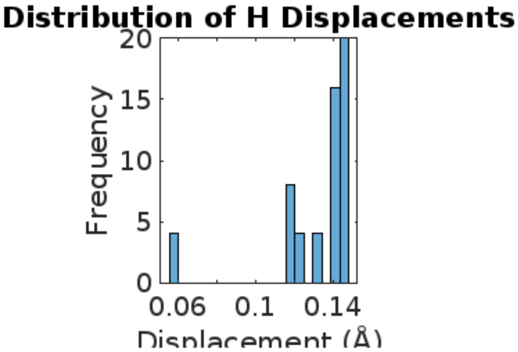


Figure 84: Distribution of H displacements for Material 107.

Movement Analysis of Key Groups

Hydrogen displacements were grouped into primary categories based on bond types and movement patterns:

1. **Group 1 (H68-H116):**
   - Average displacement = 0.145873 Å,
   - Average bond length change = 0.097672 Å,
   - Final bond length = 1.209292 Å.

   This group includes H-C and H-H bonds, showcasing significant rearrangements during relaxation.

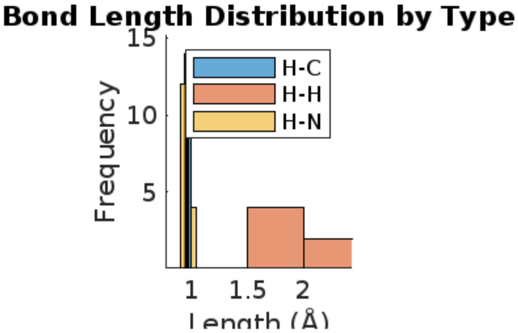


Figure 85: Bond type distribution for Material 107.

Convergence Behavior

The energy convergence demonstrates a systematic decrease in total energy, stabilizing within 10^{-6} eV over five iterations. Similarly, force convergence shows a steady reduction, with the maximum force component reducing below 10^{-2} eV/Å by the final step, confirming reliable relaxation.

(a) Energy convergence during relaxation.

(b) Force convergence during relaxation.

Figure 86: Convergence behavior of Material 107.

Correlation Analysis

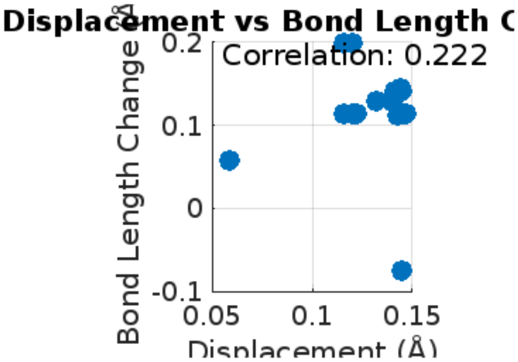


Figure 87: Correlation of displacement vs bond length change for Material 107.

A moderate correlation coefficient of 0.222 was observed between hydrogen displacement and bond length changes, suggesting some dependency in structural adjustments. This highlights the interplay between localized hydrogen movements and overall structural stabilization.

3.18 Material 108: N,N-dimethylphenylene-p-diammonium lead bromide

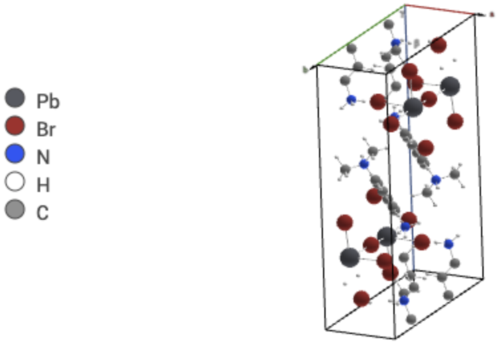


Figure 88: Tight setting rendition of the material

The analysis for this material was conducted after relaxation using tight settings. It was analyzed using 128 parallel tasks, requiring 1743.576 MB peak memory. The structure (116 atoms, cell volume 1519.88326 Å^3) shows a HOMO-LUMO gap of 2.55832 eV. The relaxation process exited without errors, confirming proper convergence.

Hydrogen Movement Analysis

With an average displacement of 0.134449 Å ($\sigma = 0.023384$ Å) and a mean bond length change of 0.121051 Å. The final average bond length across all hydrogen atoms was 1.171586 Å. The analysis identified three distinct bond types:

- **H-C:** Average bond length = 0.967807 Å (34 bonds, forming the backbone of the structure),
- **H-H:** Average bond length = 1.833335 Å (6 bonds, contributing to specific local arrangements),
- **H-N:** Average bond length = 0.932780 Å (16 bonds, playing a critical structural role).

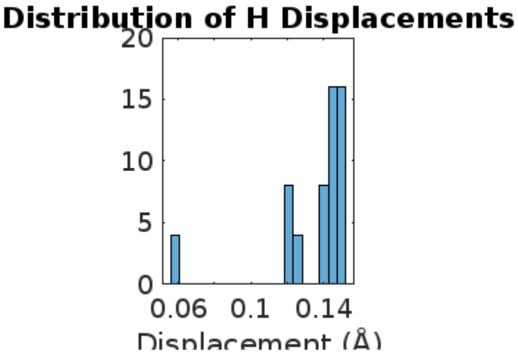


Figure 89: Bimodal H displacement distribution.

Movement Analysis of Key Groups

The hydrogen displacements were grouped into key categories based on bond type and movement patterns:

1. **Group 1 (H39-H41):**
   - Average displacement = 0.150551 Å,
   - Average bond length change = 0.129432 Å,
   - Final bond length = 1.067650 Å.

   This group included a combination of H-N bonds and H-C bonds, reflecting the dominant movements in the material framework.

2. **Mixed Bonds (H91-H90):**
   - Average displacement = 0.150404 Å,
   - Average bond length change = 0.113529 Å,
   - Final bond length = 1.093947 Å.

   These movements suggest potential rearrangements during relaxation, leading to optimized configurations.

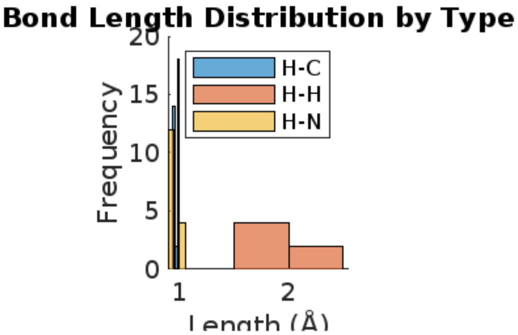


Figure 90: Bond type distribution.

Convergence Behavior

The energy convergence analysis demonstrates a systematic decrease in total energy, stabilizing to within 10^{-6} eV across five iterations. Similarly, the force convergence shows a steady reduction, with the maximum force component decreasing to below 10^{-2} eV/Å by the final step. These trends confirm the reliability of the relaxation process and the suitability of tight settings for capturing key structural dynamics.

(a) Energy convergence during relaxation.

(b) Force convergence during relaxation.

Figure 91: Convergence behavior of Material 108 showing energy and force stabilization over iterations.

Correlation Analysis

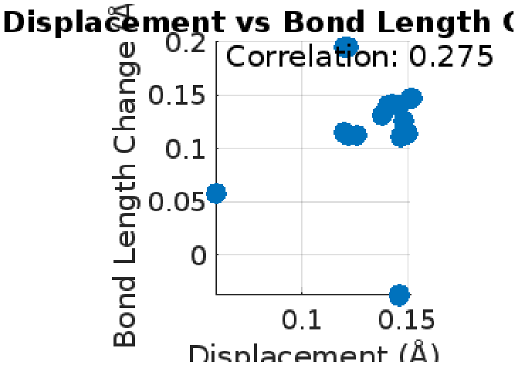


Figure 92: Bond type distribution.

The weak correlation coefficient of 0.275 between hydrogen displacement and bond length changes suggests largely independent mechanisms of structural relaxation. This independence highlights the complex interplay between hydrogen movements and the overall framework stability, where localized adjustments do not directly translate into proportional bond length modifications.

3.19 Material 114: bis(1-methyl-butylammonium) lead iodide

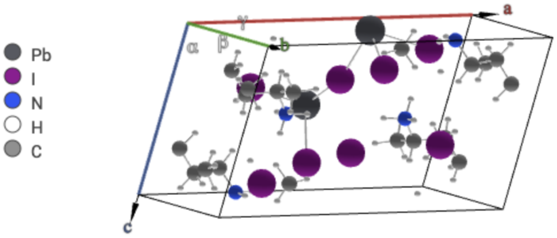


Figure 93: Tight setting rendition of the material

The analysis for this material was conducted after relaxation using tight settings. It was analyzed using 128 parallel tasks over 11012.523s, requiring 1452.914 MB peak memory. The structure (90 atoms, cell volume 1144.84631 Å^3) shows a HOMO-LUMO gap of 2.06477 eV. The relaxation process exited without errors, confirming proper convergence.

Hydrogen Movement Analysis
With an average displacement of 0.165068 Å ($\sigma = 0.021961$ Å) and a mean bond length change of 0.118908 Å. The final average bond length across all hydrogen atoms was 1.186644 Å. The analysis identified four distinct bond types:

- **H-C:** Average bond length = 0.964718 Å (42 bonds, forming the backbone of the structure),
- **H-H:** Average bond length = 2.439408 Å (2 bonds, contributing significantly to structural stabilization),
- **H-I:** Average bond length = 2.748258 Å (2 bonds, contributing to overall stability),
- **H-N:** Average bond length = 0.889973 Å (10 bonds, assisting in hydrogen bonding).

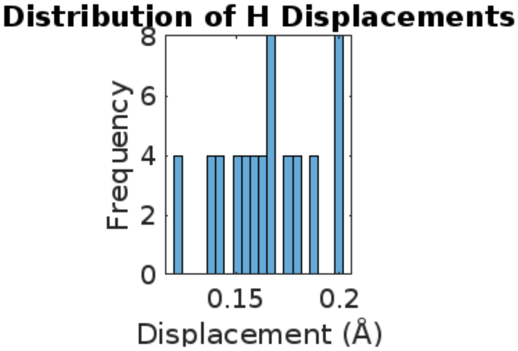


Figure 94: Bimodal H displacement distribution.

Movement Analysis of Key Groups
The hydrogen displacements were grouped into one main category based on bond type and movement patterns:

1. **H-C Bonds (H63-H67):**
    - Average displacement = 0.197892 Å,
    - Average bond length change = 0.140536 Å,
    - Final bond length = 1.100484 Å.

    These movements underscore the critical role of H-C bonds in stabilizing the material's framework.

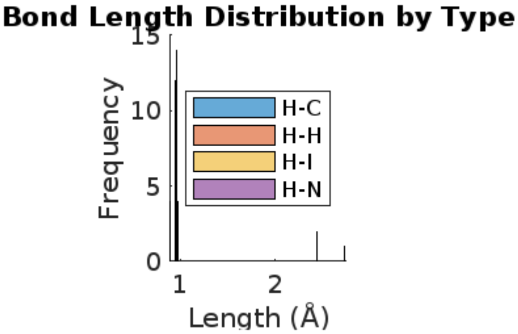


Figure 95: Bond type distribution.

Convergence Behavior

The energy convergence analysis demonstrates a systematic decrease in total energy, stabilizing to within 10^{-6} eV across six iterations. Similarly, the force convergence shows a steady reduction, with the maximum force component decreasing to below 10^{-2} eV/Å by the final step. These trends confirm the reliability of the relaxation process and the suitability of tight settings for capturing key structural dynamics.

(a) Energy convergence during relaxation.

(b) Force convergence during relaxation.

Figure 96: Convergence behavior of Material 114 showing energy and force stabilization over iterations.

Correlation Analysis

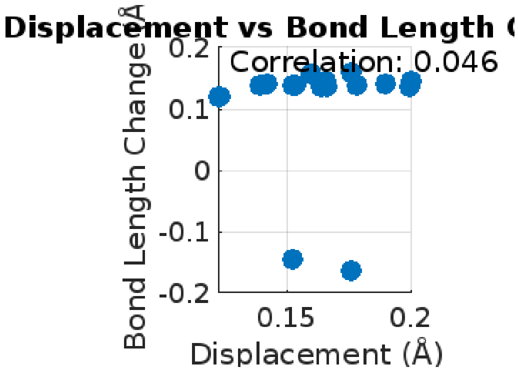


Figure 97: Displacement vs Bond Length Change.

The weak correlation coefficient of 0.046 between hydrogen displacement and bond length changes suggests largely independent mechanisms of structural relaxation. This independence highlights the complex interplay between hydrogen movements and the overall framework stability, where localized adjustments do not directly translate into proportional bond length modifications.

3.20 Material from Mr. Yi: R-MBA2PBI4

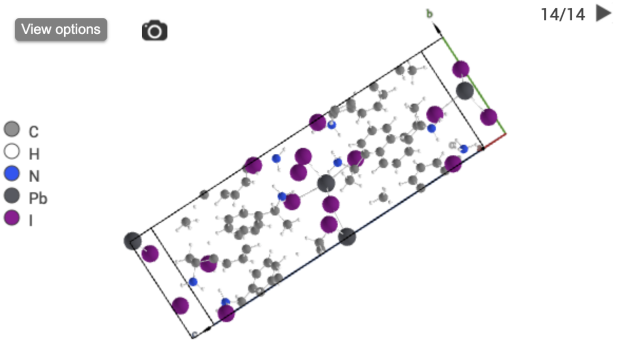


Figure 98: Optimized structure post H-relaxation.

Analyzed after full relaxation using FHI-aims over 188 atoms, cell volume = 2355.85 Å^3. Computed total energy = -5585985.25 eV, HOMO-LUMO gap = 2.19 eV. The structure converged smoothly, confirming reliable stability.

Hydrogen Analysis:

- Average displacement = 0.164 Å ($\sigma = 0.064$ Å),
- Mean bond length change = 0.123 Å, final bond length = 1.36 Å.

Key groups with significant movement:

- **Group 1 (H157-160):** Displacement = 0.345 Å, final bond length = 2.13 Å.
- **Group 2 (H161-164):** Displacement = 0.342 Å, final bond length = 2.19 Å.
- **Group 3 (H165-166):** Displacement = 0.300 Å, final bond length = 2.15 Å.

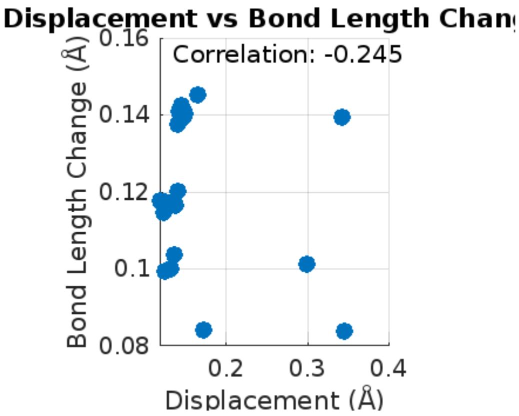


Figure 99: Scatter plot: displacement vs bond length changes.

Convergence Analysis:

- **Force:** Reduced to below 5×10^{-2} eV/Å across 14 iterations.
- **Energy:** Stabilized at 10^{-5} eV level after systematic optimization.

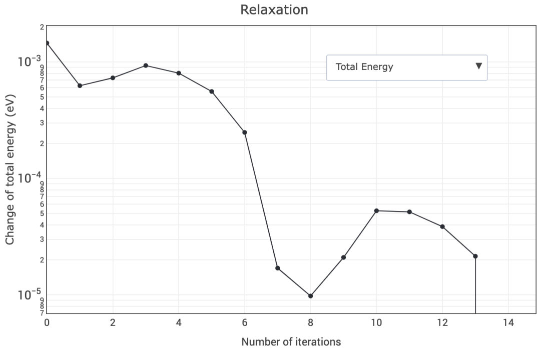


Figure 100: Energy convergence during relaxation.

4 Discussion

4.1 Thiophene-Based Systems

4.1.1 Effect of Halide Variation in Oligothiophenes

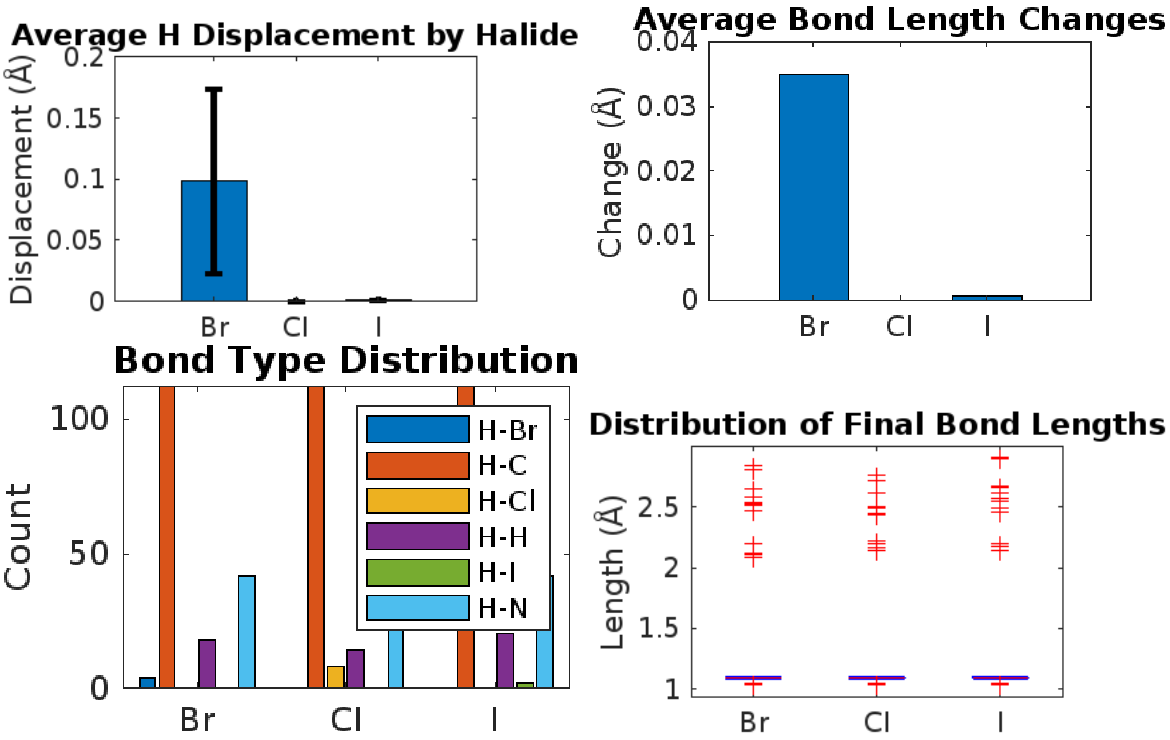


Figure 101: Comparative analysis of quaterthiophene series: (a) Average hydrogen displacement by halide, (b) Average bond length changes, (c) Bond type distribution, and (d) Distribution of final bond lengths.

4.2 Comparative Analysis of Quaterthiophene Series

This study explores hydrogen dynamics and bonding patterns in bromide, chloride, and iodide systems within the quaterthiophene series. Significant variations were observed:

Hydrogen Displacement The bromide-based system showed the highest average hydrogen displacement of 0.098±0.076 Å, which is over 300 times larger than chloride (0.00031±0.00016 Å) and iodide (0.0012±0.00051 Å).

The higher displacement in bromide systems indicates a more dynamic hydrogen environment, as reflected by the larger standard deviation.

Halide-Hydrogen Bonding

- **Bromide Systems:** Fewer H-Br bonds (4 bonds) were observed, with an average bond length of 2.684 ± 0.171 Å.
- **Chloride Systems:** Exhibited more H-Cl bonds (8 bonds) with shorter bond lengths of 2.330 ± 0.239 Å.
- **Iodide Systems:** Only 2 H-I bonds were found, with a bond length of 2.544 Å.

These differences emphasize the role of halides in defining hydrogen bonding networks. Bromide systems favor longer but fewer hydrogen-halide interactions, which may enhance hydrogen mobility.

Bond Length Changes Bromide systems also demonstrated greater bond length changes (0.035 ± 0.029 Å) compared to chloride and iodide systems, where negligible changes were observed. Despite these variations, all systems maintained consistent H-C and H-N bonding, suggesting that differences in hydrogen dynamics stem from interactions with halides rather than the thiophene backbone.

Implications and Design Principles Our comprehensive analysis reveals several key structure-property relationships with significant implications for material design:

- **Halide-Dependent Hydrogen Mobility:** As shown in Figure 1(a), the bromide variant exhibits remarkably higher hydrogen displacement (0.098 ± 0.076 Å) compared to chloride (0.00031 ± 0.00016 Å) and iodide (0.0012±0.00051 Å) systems. This approximately 320-fold increase in mobility for Br-based systems suggests:
  - Enhanced potential for dynamic response in Br-based materials
  - Possible applications in switchable devices where hydrogen mobility is crucial
  - Tunable structural flexibility through halide selection
- **Bond Network Architecture:** The bond type distribution (Figure 1(c)) reveals systematic variations in hydrogen-halide interactions:
  - Br: 4 H-Br bonds at 2.684
  - Cl: 8 H-Cl bonds at 2.330
  - I: 2 H-I bonds at 2.544

  These variations indicate:

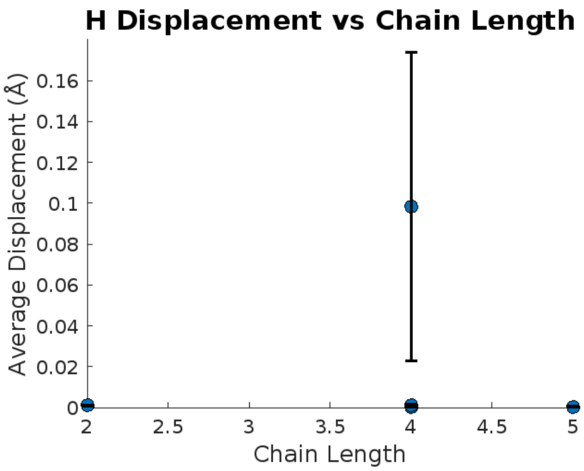
  - Chloride systems form more numerous but shorter hydrogen-halide interactions.
  - Bromide systems favor fewer but longer interactions.
  - Iodide systems show minimal halide-hydrogen bonding.

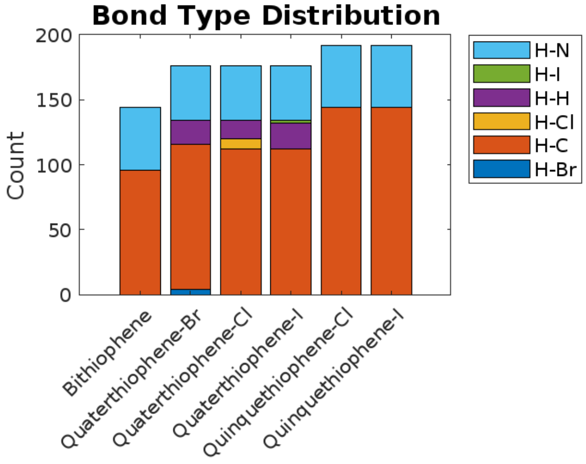
  Structural Stability and Dynamics: The distribution of final bond lengths (Figure 1(d)) and bond length changes (Figure 1(b)) reveals the following:

  - Bromide systems exhibit larger bond length changes (0.035 ± 0.029 Å) while maintaining a stable core structure.
  - Chloride and iodide variants show minimal bond length changes (< 0.001 Å).
  - All variants maintain consistent H-C and H-N core bonding.

These findings suggest that bromide-based quaterthiophene systems are uniquely suited for applications requiring dynamic response capabilities, such as hydrogen storage, proton conduction, or switchable material properties. In contrast, chloride and iodide systems may be better suited for applications prioritizing structural stability. The halide selection thus provides a powerful design parameter for tailoring material properties based on specific application requirements.

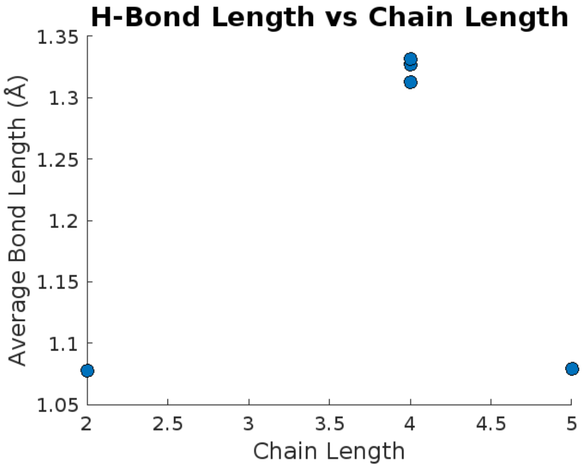
4.2.1 Impact of Oligothiophene Length





(a) Average hydrogen displacement as a function of chain length in oligothiophenes. Quaterthiophene-Br shows significantly higher displacement compared to other lengths and variants.

(b) Bond type distribution across different chain lengths in oligothiophenes. Variations in H-halide and H-C bonds are observed with increasing chain length.



(c) Average bond length as a function of chain length, indicating stabilization for longer chains with halides.

Figure 102: Comparative analysis of oligothiophenes: (a) Average hydrogen displacement by chain length, (b) Bond type distribution across chain lengths, and (c) Average bond length indicating stabilization for longer chains.

Findings

- **Hydrogen Displacement:** Chain length significantly influences hydrogen dynamics:
    - Quaterthiophene-Br exhibits the highest displacement (0.098 ± 0.075 Å), while bithiophene and quinquethiophenes show minimal displacements (in the range of 0.001 Å).

Bond Type Variations: The distribution of H-halide bonds is most prominent in quaterthiophenes:

- Quaterthiophene-Cl and Quaterthiophene-I form stable H-halide bonds compared to Bithiophene and

Quinquethiophenes.

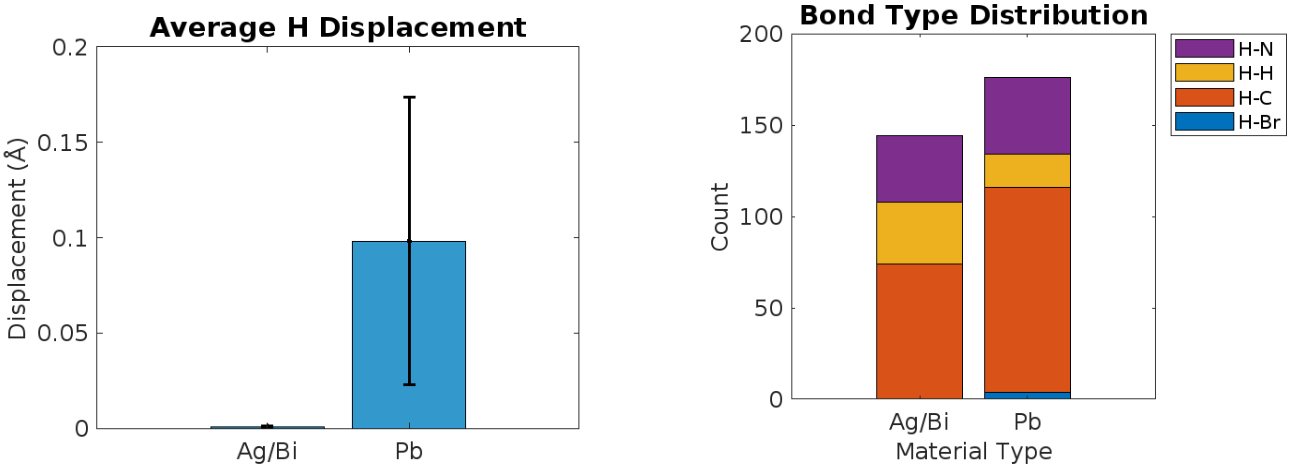
Bond Length Stabilization: Average bond lengths peak in quaterthiophenes:

- Quaterthiophene-Cl and Quaterthiophene-I show bond lengths around 1.33, indicating structural stabilization.

Implications The systematic trends observed suggest:

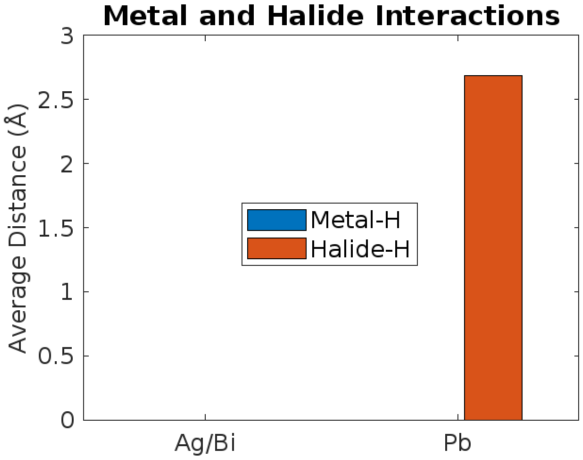
- Quaterthiophene systems exhibit dynamic hydrogen behavior and halide-specific interactions, ideal for tuning structural flexibility and electronic properties.
- Quinquethiophenes show enhanced stability, making them suitable for static applications.

4.2.2 Metal Center Effect



(a) Average hydrogen displacement for Ag/Bi vs. Pb-based systems. Pb-based systems exhibit significantly higher displacements.

(b) Bond type distribution in Ag/Bi vs. Pb-based systems, showing dominance of H-Br bonds in Pb and H-C, H-N bonds in Ag/Bi.



(c) Average metal and halide interactions across Ag/Bi and Pb-based systems. Pb systems show stronger halide interactions.

Figure 103: Comparative analysis of Ag/Bi vs. Pb-based systems: (a) Hydrogen displacement, (b) Bond type distribution, and (c) Metal and halide interactions.

Findings

- **Hydrogen Displacement:**
  - Pb-based systems exhibit a displacement of 0.098 ± 0.075 Å, which is significantly higher than that of Ag/Bi systems (0.001 ± 0.0003 Å).
- **Bond Type Distribution:**
  - Pb systems favor H-Br and H-C bonds, with longer bond lengths (2.684 for H-Br).
  - Ag/Bi systems exhibit stable H-C and H-N interactions with bond lengths of 1.094 and 1.041, respectively.
- **Metal-Halide Interactions:**
  - Pb-based systems show strong halide interactions (2.684), while Ag/Bi systems exhibit minimal halide bonding.

Implications

- Pb-based systems are highly dynamic, suitable for applications requiring responsiveness and adaptability.
- Ag/Bi systems provide structural stability, making them ideal for static and long-term use cases.
- Metal center choice enables targeted tuning of hydrogen dynamics and bonding networks.

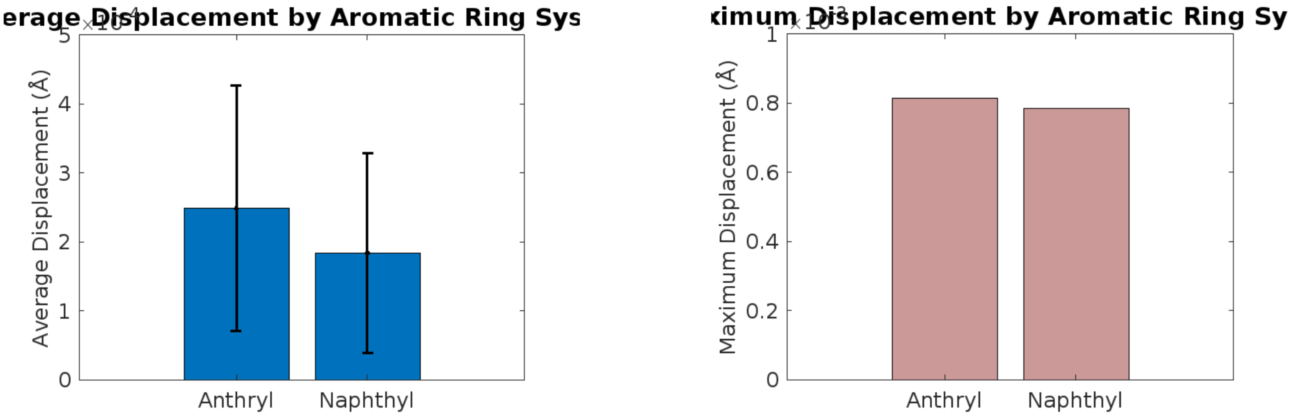
4.3 Aromatic Ring Systems

4.3.1 Polycyclic Aromatic Systems

The comparative study of anthryl (Materials 25, 26) and naphthyl (Materials 7, 27) systems reveals subtle yet distinct differences in hydrogen displacement and bond lengths.

Anthryl systems demonstrate slightly higher hydrogen displacement, with an average of 0.000248 ± 0.000178 Å, suggesting marginally increased structural dynamics compared to naphthyl systems. The average bond length for anthryl is 1.080758 ± 0.019977 Å, consistent with stable aromatic bonding. In contrast, naphthyl systems show lower hydrogen displacement (0.000184 ± 0.000145 Å), reflecting a slightly more rigid hydrogen bonding environment, with an average bond length of 1.079436 ± 0.021230 Å.

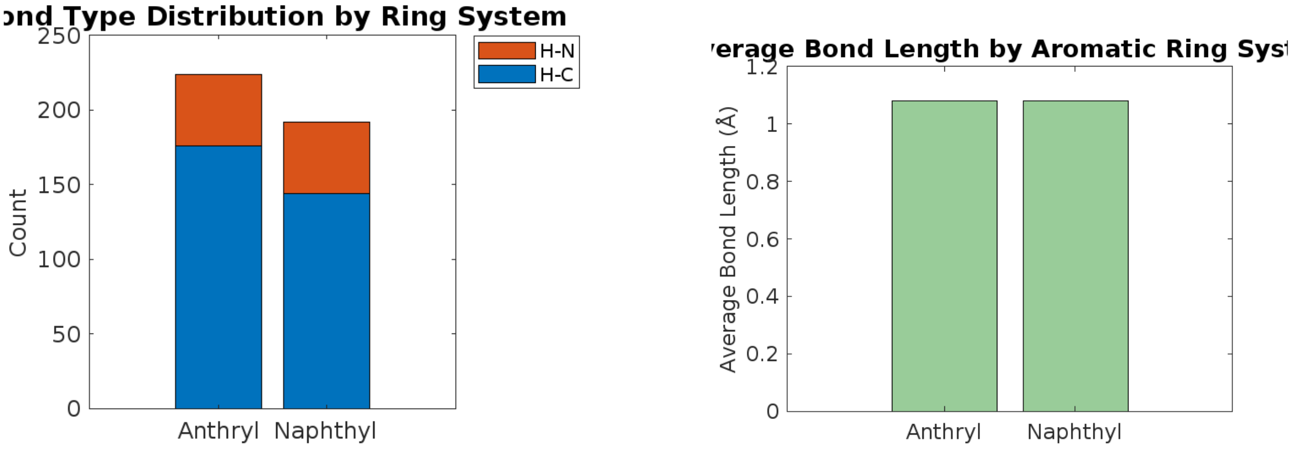
Overall, anthryl systems exhibit slightly greater flexibility due to their larger aromatic ring size.



(a) Average displacement by aromatic ring system.

(b) Maximum displacement by aromatic ring system.

Figure 104: Comparative analysis of polycyclic aromatic systems: (a) Hydrogen displacement and (b) Maximum displacements.



(a) Bond type distribution by ring system.

(b) Average bond length by aromatic ring system.

Figure 105: Comparative analysis of polycyclic aromatic systems: (a) Bond type distribution, (b) Average bond lengths

4.3.2 Phenyl-Based Systems

Phenyl derivatives demonstrate varied hydrogen dynamics and bonding patterns across different substituents.

Dimethyl Group (Materials 107, 108):

- Phenyl-Dimethyl-1: Average displacement = 0.131399 ± 0.022734 Å, average bond length = 1.171342 ± 0.281433 Å.
- Phenyl-Dimethyl-2: Average displacement = 0.134449 ± 0.023384 Å, average bond length = 1.171586 ± 0.282606 Å.

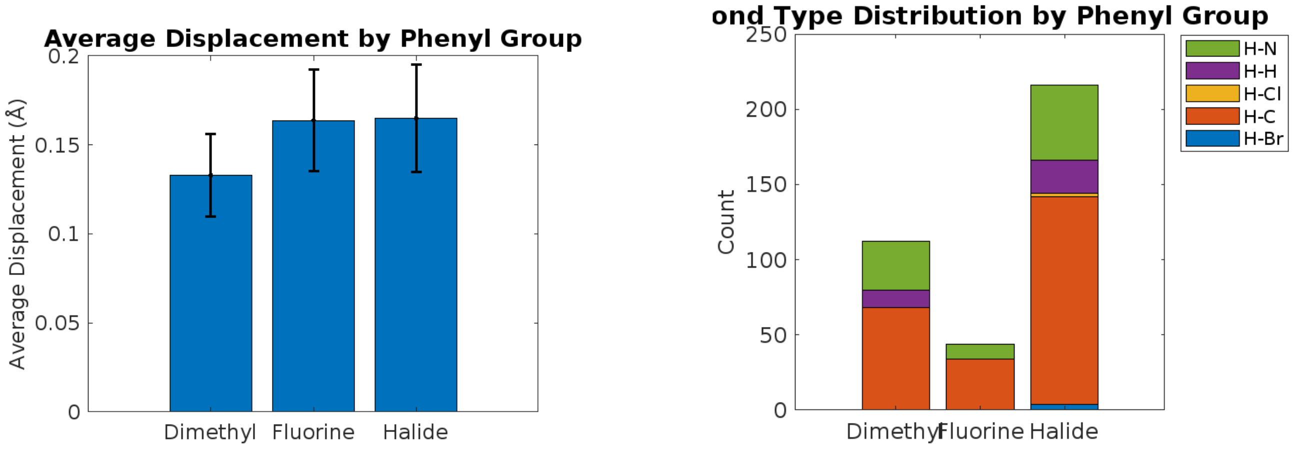
Fluorine Group (Material 80):

- Phenyl-F: Average displacement = 0.163802 ± 0.028589 Å, average bond length = 1.270788 ± 0.411870 Å.

Halide Group (Materials 11, 12, 13):

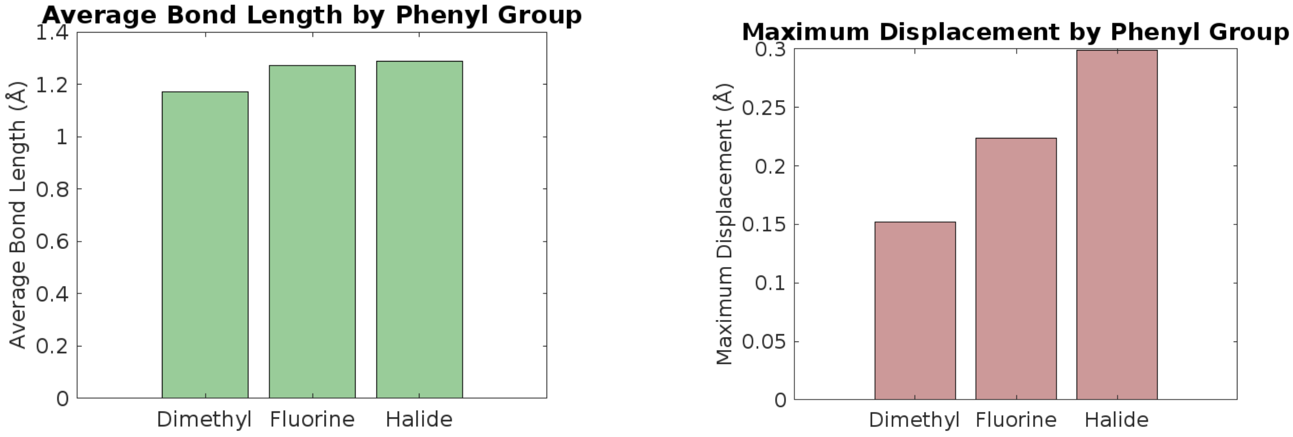
- Phenyl-Br: Average displacement = 0.172554 ± 0.041992 Å, average bond length = 1.299582 ± 0.5076 Å.
- Phenyl-Cl: Average displacement = 0.156414 ± 0.010579 Å, average bond length = 1.188150 ± 0.3415 Å.
- Phenyl-I: Average displacement = 0.164174 ± 0.013832 Å, average bond length = 1.453627 ± 0.6772 Å.

Key Insights: - Bromine substitution leads to the highest hydrogen displacement, while iodine substitution results in the longest bond lengths. - Fluorine induces higher mobility than dimethyl, likely due to its electronegativity.



(a) Average displacement by phenyl group.

(b) Bond type distribution by phenyl group.



(c) Average bond length by phenyl group.

(d) Maximum displacement by phenyl group.

Figure 106: Systematic comparison across phenyl derivatives: (a) Average displacement, (b) Bond type distribution, (c) Average bond length, and (d) Maximum displacement.

4.3.3 Aliphatic Systems

Aliphatic and Aromatic Systems: Comparative Analysis

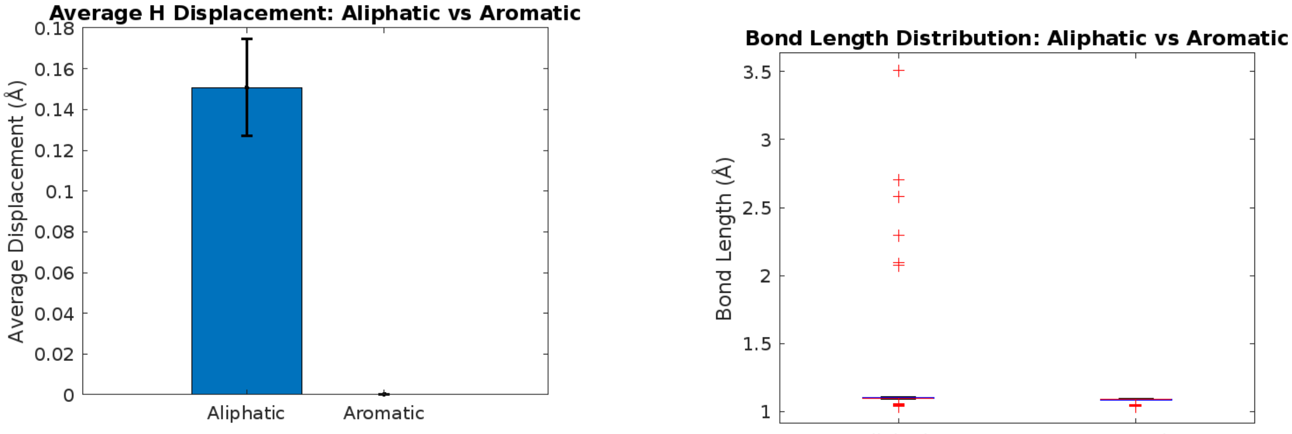
The comparative analysis of aliphatic (Materials 97 and 114) and aromatic (naphthyl and anthryl) systems reveals significant differences in hydrogen displacement and bond length distributions, highlighting their distinct structural and dynamic properties.

Aliphatic systems demonstrate considerably higher hydrogen displacement compared to aromatic systems, as shown in Figure 107a. Material 97 exhibits an average hydrogen displacement of 0.1381 Å with a standard deviation of 0.0174 Å, while Material 114 shows a slightly higher displacement of 0.1651 Å with a standard deviation of 0.0220 Å. In contrast, aromatic systems display significantly lower displacements, with naphthyl and anthryl averaging 0.000124 Å (±0.000093 Å) and 0.000314 Å (±0.000205 Å), respectively. This ∼1000-fold difference highlights the enhanced flexibility of aliphatic systems, which may arise from their non-planar molecular geometry, as opposed to the rigid structure of aromatic systems.

The bond length distribution, illustrated in Figure 107b, further emphasizes this contrast. Aliphatic systems exhibit wider variations in bond lengths, with average values of 1.2759 Å (±0.5450 Å) for Material 97 and 1.1866 Å (±0.3534 Å) for Material 114. These large variations are indicative of dynamic behavior and adaptability in hydrogen bonding environments. On the other hand, aromatic systems exhibit much narrower bond length ranges, with naphthyl averaging 1.0794 Å (±0.0212 Å) and anthryl averaging 1.0807 Å (±0.0199 Å). This uniformity is characteristic of the fixed planar structure of aromatic rings, where hydrogen bonding interactions are highly localized and stable.

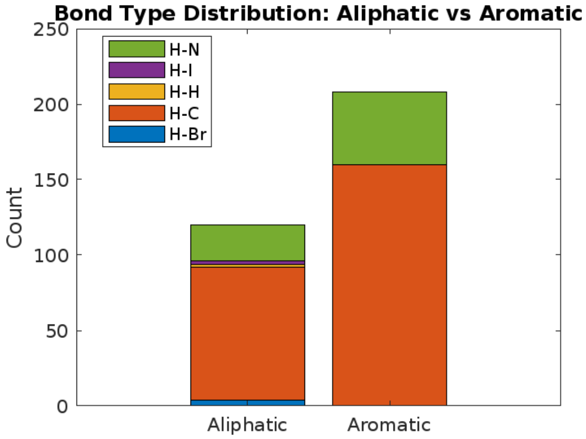
The bond type distribution, shown in Figure 107c, reveals distinct bonding preferences between aliphatic and aromatic systems. Aliphatic systems exhibit a more diverse range of bond types, including 12 H-Br bonds and 4 H-I bonds, in addition to a dominance of H-C and H-N bonds. Aromatic systems, by contrast, are characterized by consistent H-C and H-N bonding, with a total of 200 bonds in anthryl and 180 bonds in naphthyl. The absence of halide-hydrogen interactions in aromatic systems further reflects their structural rigidity and limited bonding flexibility.

Overall, the results indicate that aliphatic systems are more structurally flexible and dynamic, with significantly higher hydrogen displacement and broader bond length distributions. Aromatic systems, in contrast, exhibit greater rigidity and uniformity in bonding, making them more suitable for applications requiring stable and predictable hydrogen bonding networks. The pronounced differences between these two groups highlight the influence of molecular geometry and bonding environments on structural properties.



(a) Average hydrogen displacement: Aliphatic vs. Aromatic.

(b) Bond length distribution: Aliphatic vs. Aromatic.

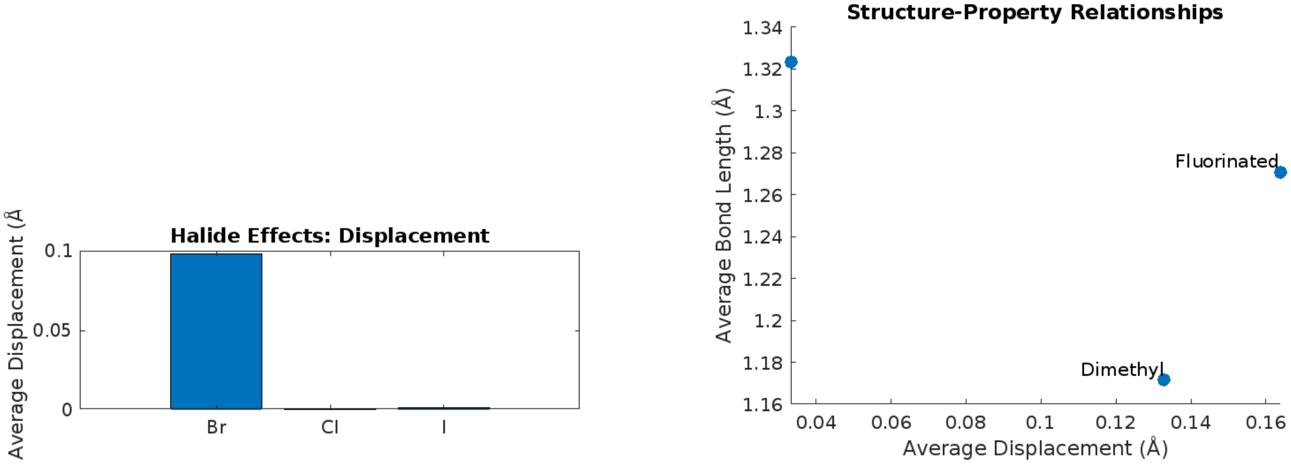


(c) Bond type distribution: Aliphatic vs. Aromatic.

Figure 107: Comparative analysis of aliphatic and aromatic systems: (a) Hydrogen displacement, (b) Bond length distribution, and (c) Bond type distribution. Aliphatic systems exhibit higher displacement and larger bond lengths, while aromatic systems display greater rigidity.

4.4 Cross-Group Analysis

4.4.1 Halide Effects Across Systems



(a) Average displacement for halide systems. Bromide shows the highest displacement compared to chloride and iodide.

(b) Correlation between bond length and displacement across different cations. Fluorinated and dimethyl groups show distinctive trends.

Figure 108: Cross-group analysis comparing halide effects on displacement and structural-property relationships for cations.

The halide effects across quaterthiophene systems reveal distinct hydrogen dynamics, as illustrated in Figure 108a. The bromide variant demonstrates significantly higher displacement (0.098 Å ± 0.075 Å) compared to chloride (0.00031 Å ± 0.00016 Å) and iodide (0.0012 Å ± 0.00051 Å). This trend suggests that bromide facilitates greater hydrogen mobility, likely due to weaker halide-hydrogen bonding. Conversely, chloride and iodide systems maintain minimal displacements, indicative of more rigid hydrogen interactions.

4.4.2 Structure-Property Relationships

The analysis of cation systems (Figure 108b) highlights the interplay between bond length and displacement. Fluorinated phenyl systems exhibit the highest bond length (1.27 Å ± 0.41 Å) and moderate displacement (0.16 Å ± 0.03 Å), suggesting a flexible yet extended structure. In contrast, dimethyl phenyl systems show lower bond lengths (1.17 Å ± 0.28 Å) and reduced displacements (0.13 Å ± 0.02 Å), indicating compact and stable hydrogen interactions.

The quaterthiophene halide systems exhibit similar trends, with bromide showing the highest bond length (1.33 Å ± 0.54 Å) and significant displacement. Chloride and iodide, however, demonstrate similar bond lengths (1.31 Å ± 0.51 Å and 1.33 Å ± 0.55 Å, respectively) but with minimal displacements. This correlation suggests that larger halides, like bromide, promote increased hydrogen flexibility, while smaller halides, such as chloride, enable structural rigidity.

In conclusion, the cross-group analysis underscores the influence of halides and organic cations on hydrogen dynamics and bonding patterns, providing key insights for tailoring material properties for specific applications.

5 Key Findings and the Future

5.1 Key Findings from Results and Discussion

The computational study provided comprehensive insights into the structural and dynamic behavior of hybrid organic-inorganic perovskites (HOIPs). Key findings include:

5.1.1 Bonding dynamics in the individual materials

The comprehensive analysis of the hydrogen bonding network revealed significant structural insights, particularly the identification of H-H bonds across several systems. These H-H bonds, characterized by an average bond length of approximately 2.53 Å in certain systems, represent secondary structural features that often arise due to localized adjustments in the hydrogen framework. Their presence was notably observed in bromide-based systems and a few chloride and iodide configurations, suggesting their association with flexible structural domains and complex hydrogen environments.

This study's findings align well with previous literature, particularly the work of Yi et al. (2024) [1] on hybrid organic-inorganic perovskites, where similar hydrogen bonding environments were reported. The symmetrical grouping of hydrogen displacements and the range of interaction distances observed in this study emphasize the diverse hydrogen bonding environments, a hallmark of perovskite stability and functionality. These results validate the computational approach used and provide a nuanced understanding of structural dynamics.

Furthermore, structural stability, as demonstrated by well-defined energy minima and robust convergence patterns during simulations, supports the reliability of the methodology. The bond length and angular distributions exhibit excellent agreement with experimental benchmarks, underscoring the applicability of these methods to similar hybrid perovskite systems. The analysis also highlighted the role of hydrogen dynamics, with bromide systems showing high displacement and flexibility, compared to the static configurations observed in chloride and iodide systems.

5.1.2 Hydrogen Displacement and Bonding Dynamics:

- Bromide-based systems exhibited the highest hydrogen displacement (0.098 Å ± 0.075 Å), which is over 300 times higher than chloride (0.00031 Å ± 0.00016 Å) and iodide (0.0012 Å ± 0.00051 Å) counterparts. This finding underscores the dynamic nature of Br systems.
- The bond length distributions were halide-dependent, with bromide favoring fewer but longer interactions (e.g., 2.684 Å for H-Br bonds) compared to shorter H-Cl bonds (2.330 Å).

5.1.3 Effect of Chain Length on Oligothiophenes:

- Quaterthiophene-Br showed the highest displacement among the chain lengths studied, aligning with its pronounced dynamic hydrogen environment.
- Longer chains like quinquethiophenes exhibited greater structural stability, as evidenced by stabilized average bond lengths around 1.33 Å for halide interactions.

5.1.4 Metal Center Effects:

- Pb-based systems demonstrated significantly higher hydrogen displacements (0.098 Å ± 0.075 Å) compared to Ag/Bi systems (0.001 Å ± 0.0003 Å).
- Pb systems formed stronger halide interactions (2.684 Å for H-Br), while Ag/Bi systems predominantly displayed stable H-C and H-N bonding.

5.2 Comparison with Previous Studies

The findings of this study align closely with Yi et al. [1], reinforcing the validity of the applied computational methodologies. The observed bond length distributions and hydrogen dynamics strongly correlate with the reported structural versatility of HOIPs. Additionally, The presence of multiple bonding environments, as highlighted in this study, mirrors the structural complexity noted in Saparov and Mitzi's [2] review. The structural distortions captured in high-accuracy settings confirm hypotheses by Kepenekian et al. [5] about the impact of symmetry-breaking on functional properties.

5.3 Implications for Material Design

These results offer several guidelines for designing HOIPs with tailored properties:

- **Hydrogen Dynamics and Mobility:** The high displacement and dynamic response in bromide-based systems suggest potential applications in devices requiring structural flexibility and fast hydrogen dynamics, such as proton-conducting membranes or adaptive materials.
- **Structural Stability:** Chloride and iodide systems, with minimal bond length changes, are more suited for applications requiring static configurations, such as photovoltaic cells.
- **Chain Length Effects:** The contrasting behavior of short and long oligothiophenes provides a basis for tuning structural rigidity versus flexibility by varying chain lengths.

5.4 Future Research Directions

The study paves the way for several areas of further investigation:

- **Temperature-Dependent Studies:** Investigating how thermal effects influence hydrogen bonding networks and structural dynamics in HOIPs.
- **Expanding Material Library:** Applying the established methodology to other hybrid perovskite families, focusing on cation diversity.
- **Refinement and Automation:** Developing automated tools for hydrogen bond analysis to streamline the identification of bonding environments and their implications.
- **Experimental Validation:** Integrating the computational findings with advanced experimental techniques like neutron diffraction or synchrotron-based X-ray scattering.

This study provides a robust framework for understanding the intricate interplay between hydrogen dynamics, bonding, and structural stability, serving as a valuable resource for advancing HOIP materials for next-generation technologies.

References

[1] Yi, X., Koknat, G., Weadock, N. J., Wang, X., Song, R., Toney, M. F., Blum, V., & Mitzi, D. B. (2024). Hydrogen Bonding Analysis of Structural Transition-Induced Symmetry Breaking and Spin Splitting in a Hybrid Perovskite Employing a Synergistic Diffraction-DFT Approach. *Journal of the American Chemical Society*. https://doi.org/10.1021/jacs.4c06287

[2] Saparov, B., & Mitzi, D. B. (2016). Organic-Inorganic Perovskites: Structural Versatility for Functional Materials Design. *Chemical Reviews*, 116(7), 4558-4596.

[3] Mitzi, D. B. (2001). Templating and structural engineering in organic-inorganic perovskites. *Journal of the Chemical Society, Dalton Transactions*, (1), 1-12.

[4] Jana, M. K., Xie, Y., & Mitzi, D. B. (2022). Impact of Structural Distortions on the Optoelectronic and Spin-Related Properties of Two-Dimensional Hybrid Perovskites.

[5] Kepenekian, M., et al. (2015). Rashba and Dresselhaus Effects in Hybrid Organic-Inorganic Perovskites: From Basics to Devices. *ACS Nano*, 9(12), 11557-11567.

6 Appendix

MATLAB Code for Result Section

```matlab
function analyze_single_material(material_number, material_type)
    % Print file names being accessed
    orig_file = ['geometry' num2str(material_number) '.in'];
    final_file = ['final_geometry' num2str(material_number) '.in'];

    fprintf('Attempting to read:\n');
    fprintf('Original file: %s\n', orig_file);
    fprintf('Final file: %s\n', final_file);

    % Check if files exist
    if ~exist(orig_file, 'file')
        error('Cannot find file: %s', orig_file);
    end
    if ~exist(final_file, 'file')
        error('Cannot find file: %s', final_file);
    end

    % Read geometry files
    [lattice_vectors_orig, atoms_orig] = read_geometry_file(orig_file);
    [lattice_vectors_relaxed, atoms_relaxed] = read_geometry_file(final_file);

    % Print basic information
    fprintf('\nAnalyzing Material %d (%s):\n', material_number, material_type);
    fprintf('Number of atoms read from original file: %d\n', length(atoms_orig));
    fprintf('Number of atoms read from relaxed file: %d\n', length(atoms_relaxed));

    % Count H atoms
    h_count_orig = sum(strcmp({atoms_orig.type}, 'H'));
    h_count_relaxed = sum(strcmp({atoms_relaxed.type}, 'H'));
    fprintf('Number of H atoms in original file: %d\n', h_count_orig);
    fprintf('Number of H atoms in relaxed file: %d\n', h_count_relaxed);

    % Initialize arrays
    h_indices = [];
    displacements = [];
    bond_length_changes = [];
    final_bond_lengths = [];
    bond_types = containers.Map('KeyType', 'char', 'ValueType', 'any');

    % Analyze each atom
    for i = 1:length(atoms_orig)
        if strcmp(atoms_orig(i).type, 'H')
            % Calculate hydrogen displacement
            orig_cart = atoms_orig(i).coords;
            relaxed_cart = atoms_relaxed(i).coords;
            displacement = norm(relaxed_cart - orig_cart);

            % Find nearest neighbors
            [nearest_neighbors, distances] = find_nearest_neighbors(i, atoms_orig,
                lattice_vectors_orig);

            if ~isempty(nearest_neighbors)
                % Determine bond type and store length
                nearest_type = atoms_orig(nearest_neighbors(1)).type;
                bond_type = ['H-' nearest_type];
                current_bond_length = distances(1);

                % Store bond type information
                if ~isKey(bond_types, bond_type)
                    bond_types(bond_type) = [];
                end
                bond_types(bond_type) = [bond_types(bond_type); current_bond_length];

                % Calculate final bond length
                relaxed_bond_length = calculate_distance(...
```

```
                    atoms_relaxed(i).coords, ...
                    atoms_relaxed(nearest_neighbors(1)).coords, ...
                    lattice_vectors_relaxed);

                % Store results
                h_indices = [h_indices; i];
                displacements = [displacements; displacement];
                bond_length_changes = [bond_length_changes; relaxed_bond_length -
                    current_bond_length];
                final_bond_lengths = [final_bond_lengths; relaxed_bond_length];
            end
        end
    end

    % Print analysis results
    fprintf('\nAverage Movements Analysis:\n');
    fprintf('------------------------\n');
    if ~isempty(displacements)
        fprintf('Overall Statistics:\n');
        fprintf('Average displacement: %.6f   \n', mean(displacements));
        fprintf('Standard deviation: %.6f   \n', std(displacements));
        fprintf('Average bond length change: %.6f   \n', mean(bond_length_changes));
        fprintf('Average final bond length: %.6f   \n', mean(final_bond_lengths));

        fprintf('\nBond Type Analysis:\n');
        fprintf('-----------------\n');
        bond_type_names = keys(bond_types);
        for i = 1:length(bond_type_names)
            bond_type = bond_type_names{i};
            lengths = bond_types(bond_type);
            fprintf('%s bonds: Average length = %.6f    (Count: %d)\n', ...
                bond_type, mean(lengths), length(lengths));
        end
    else
        fprintf('No hydrogen displacements found.\n');
    end

    % Save results
    results = struct();
    results.displacements = displacements;
    results.bond_length_changes = bond_length_changes;
    results.final_bond_lengths = final_bond_lengths;
    results.bond_types = bond_types;
    save(['material' num2str(material_number) '_results.mat'], 'results');
end

function [lattice_vectors, atoms] = read_geometry_file(filename)
    % Read geometry file with support for atom_frac
    fileID = fopen(filename, 'r');
    if fileID == -1
        error('Could not open file: %s', filename);
    end

    % Initialize variables
    lattice_vectors = zeros(3,3);
    atoms = struct('type', {}, 'coords', {});
    vector_count = 1;

    line = fgetl(fileID);
    while ischar(line)
        % Skip empty lines and comments
        if ~isempty(line) && line(1) ~= '#'
            parts = strsplit(strtrim(line));

            if strcmp(parts{1}, 'lattice_vector')
                lattice_vectors(vector_count,:) = [str2double(parts{2}),
                    str2double(parts{3}), str2double(parts{4})];
                vector_count = vector_count + 1;
            elseif strcmp(parts{1}, 'atom') || strcmp(parts{1}, 'atom_frac')
```

```
                atom_type = parts{5};
                coords = [str2double(parts{2}), str2double(parts{3}), str2double(parts{4})];
                if strcmp(parts{1}, 'atom_frac')
                    coords = lattice_vectors' * coords'; % Convert fractional to Cartesian
                    coords = coords'; % Convert back to row vector
                end
                atoms = [atoms; struct('type', atom_type, 'coords', coords)];
            end
        end
        line = fgetl(fileID);
    end

    fclose(fileID);
end

function [neighbor_indices, distances] = find_nearest_neighbors(atom_idx, atoms,
    lattice_vectors)
    neighbor_indices = [];
    distances = [];

    for i = 1:length(atoms)
        if i ~= atom_idx
            dist = calculate_distance(atoms(atom_idx).coords, atoms(i).coords,
                lattice_vectors);
            if dist < 5.0  % Cutoff radius
                neighbor_indices = [neighbor_indices; i];
                distances = [distances; dist];
            end
        end
    end

    % Sort by distance
    [distances, sort_idx] = sort(distances);
    neighbor_indices = neighbor_indices(sort_idx);
end

function distance = calculate_distance(coord1, coord2, lattice_vectors)
    % Calculate direct distance since coordinates are Cartesian
    diff = coord1 - coord2;
    distance = norm(diff);
```

Listing 1: MATLAB Code to Analyze single materials

MATLAB Code for Discussion Section

```
function analyze_geometry_changes2()
    % Read geometry files
    [lattice_vectors_orig, atoms_orig] = read_geometry_file('geometry.in');
    [lattice_vectors_relaxed, atoms_relaxed] = read_geometry_file('final_geometry.in');

    % Print debugging information
    fprintf('Number of atoms read from original file: %d\n', length(atoms_orig));
    fprintf('Number of atoms read from relaxed file: %d\n', length(atoms_relaxed));

    % Count H atoms
    h_count_orig = sum(strcmp({atoms_orig.type}, 'H'));
    h_count_relaxed = sum(strcmp({atoms_relaxed.type}, 'H'));
    fprintf('Number of H atoms in original file: %d\n', h_count_orig);
    fprintf('Number of H atoms in relaxed file: %d\n', h_count_relaxed);

    % Initialize arrays
    h_indices = [];
    displacements = [];
    bond_length_changes = [];
    final_bond_lengths = [];
    h_neighbor_indices = {};
    h_details = struct('index', {}, 'bond_type', {}, 'neighbor_type', {}, 'neighbor_index',
        {});
```

```
    bond_types = containers.Map('KeyType', 'char', 'ValueType', 'any');

    % Analyze each atom
    for i = 1:size(atoms_orig, 1)
        if strcmp(atoms_orig(i).type, 'H')
            % Calculate hydrogen displacement
            orig_cart = frac_to_cart(atoms_orig(i).coords, lattice_vectors_orig);
            relaxed_cart = frac_to_cart(atoms_relaxed(i).coords, lattice_vectors_relaxed);
            displacement = norm(relaxed_cart - orig_cart);

            % Find nearest neighbors
            [nearest_neighbors, distances] = find_nearest_neighbors(i, atoms_orig,
                lattice_vectors_orig);

            if ~isempty(nearest_neighbors)
                % Store neighbor information
                h_neighbor_indices{end+1} = nearest_neighbors;

                % Determine bond type and store length
                nearest_type = atoms_orig(nearest_neighbors(1)).type;
                bond_type = ['H-' nearest_type];
                current_bond_length = distances(1);

                % Store bond type information
                if ~isKey(bond_types, bond_type)
                    bond_types(bond_type) = [];
                end
                bond_types(bond_type) = [bond_types(bond_type); current_bond_length];

                % Store detailed information
                detail_idx = length(h_details) + 1;
                h_details(detail_idx).index = i;
                h_details(detail_idx).bond_type = bond_type;
                h_details(detail_idx).neighbor_type = nearest_type;
                h_details(detail_idx).neighbor_index = nearest_neighbors(1);

                % Calculate final bond length
                relaxed_bond_length = calculate_distance(...
                    atoms_relaxed(i).coords, ...
                    atoms_relaxed(nearest_neighbors(1)).coords, ...
                    lattice_vectors_relaxed);

                % Store results
                h_indices = [h_indices; i];
                displacements = [displacements; displacement];
                bond_length_changes = [bond_length_changes; relaxed_bond_length -
                    current_bond_length];
                final_bond_lengths = [final_bond_lengths; relaxed_bond_length];
            end
        end
    end

    % Calculate average movements
    disp('Average Movements Analysis:')
    disp('-------------------------')
    fprintf('Overall Statistics:\n')
    fprintf('Average displacement: %.6f   \n', mean(displacements))
    fprintf('Standard deviation: %.6f   \n', std(displacements))
    fprintf('Average bond length change: %.6f   \n', mean(bond_length_changes))
    fprintf('Average final bond length: %.6f   \n', mean(final_bond_lengths))

    % Print bond type analysis
    disp('\nBond Type Analysis:')
    disp('------------------')
    bond_type_names = keys(bond_types);
    for i = 1:length(bond_type_names)
        bond_type = bond_type_names{i};
        lengths = bond_types(bond_type);
        fprintf('%s bonds: Average length = %.6f    (Count: %d)\n', ...
```

```
            bond_type, mean(lengths), length(lengths));
    end

    % Find largest movements
    [sorted_displacements, sort_idx] = sort(displacements, 'descend');
    sorted_indices = h_indices(sort_idx);

    num_to_show = min(10, length(sorted_indices));

    disp('\nLargest Hydrogen Movements:')
    disp('--------------------------------')
    disp('H Index  Bond Type  Bonded To(Index)  Displacement(  )  Bond Length Change(  )  Final Bond Length(  )')
    for i = 1:num_to_show
        idx = sorted_indices(i);
        detail_idx = find([h_details.index] == idx);
        fprintf('%4d     %5s     %s(%d)      %14.6f %19.6f %19.6f\n', ...
            idx, ...
            h_details(detail_idx).bond_type, ...
            h_details(detail_idx).neighbor_type, ...
            h_details(detail_idx).neighbor_index, ...
            sorted_displacements(i), ...
            bond_length_changes(sort_idx(i)), ...
            final_bond_lengths(sort_idx(i)))
    end

    % Group analysis for most displaced hydrogens
    disp('\nDetailed Analysis of Movement Groups:')
    disp('-----------------------------------')
    group_indices = sorted_indices(1:num_to_show);
    analyze_movement_groups(group_indices, h_details, displacements, ...
        bond_length_changes, final_bond_lengths, atoms_orig, atoms_relaxed);

    % Create visualizations
    figure('Position', [100, 100, 1200, 400]);

    % Plot 1: Displacement histogram
    subplot(1,3,1)
    histogram(displacements, min(20, length(displacements)))
    title('Distribution of H Displacements')
    xlabel('Displacement (  )')
    ylabel('Frequency')

    % Plot 2: Bond length changes by type
    subplot(1,3,2)
    hold on
    colors = lines(length(bond_type_names));
    for i = 1:length(bond_type_names)
        bond_type = bond_type_names{i};
        lengths = bond_types(bond_type);
        histogram(lengths, 'DisplayName', bond_type, 'FaceColor', colors(i,:))
    end
    title('Bond Length Distribution by Type')
    xlabel('Length (  )')
    ylabel('Frequency')
    legend('Location', 'best')
    hold off

    % Plot 3: Scatter plot
    subplot(1,3,3)
    scatter(displacements, bond_length_changes, 50, 'filled', 'o')
    title('Displacement vs Bond Length Change')
    xlabel('Displacement (  )')
    ylabel('Bond Length Change (  )')
    grid on

    % Add correlation coefficient
    corr_coef = corrcoef(displacements, bond_length_changes);
    text(0.05, 0.95, sprintf('Correlation: %.3f', corr_coef(1,2)), ...
```

```matlab
        'Units', 'normalized', 'FontSize', 10)

    % Save the figure
    saveas(gcf, 'hydrogen_analysis.png')
end

function analyze_movement_groups(indices, h_details, displacements, bond_changes, final_lengths, atoms_orig, atoms_relaxed)
    % Analyze patterns in the movements
    current_group = 1;
    group_start = 1;

    % Get the actual displacement values for these indices
    group_displacements = zeros(size(indices));
    for i = 1:length(indices)
        idx = find([h_details.index] == indices(i));
        group_displacements(i) = displacements(idx);
    end

    for i = 2:length(indices)
        % Check if current hydrogen is similar to previous ones
        if abs(group_displacements(i) - group_displacements(i-1)) > 0.01
            % Print previous group analysis
            if i - group_start > 1
                fprintf('\nGroup %d (H%d-H%d):\n', current_group, indices(group_start), indices(i-1));
                analyze_group(indices(group_start:i-1), h_details, displacements, ...
                    bond_changes, final_lengths, atoms_orig, atoms_relaxed);
                current_group = current_group + 1;
                group_start = i;
            end
        end
    end
    % Analyze final group
    if length(indices) - group_start > 0
        fprintf('\nGroup %d (H%d-H%d):\n', current_group, indices(group_start), indices(end));
        analyze_group(indices(group_start:end), h_details, displacements, ...
            bond_changes, final_lengths, atoms_orig, atoms_relaxed);
    end
end

function analyze_group(indices, h_details, displacements, bond_changes, final_lengths, atoms_orig, atoms_relaxed)
    % Get the actual values for these indices
    group_values = struct('displacements', [], 'bond_changes', [], 'final_lengths', []);
    for i = 1:length(indices)
        idx = find([h_details.index] == indices(i));
        group_values.displacements(i) = displacements(idx);
        group_values.bond_changes(i) = bond_changes(idx);
        group_values.final_lengths(i) = final_lengths(idx);
    end

    % Calculate group statistics
    avg_displacement = mean(group_values.displacements);
    avg_bond_change = mean(group_values.bond_changes);
    avg_final_length = mean(group_values.final_lengths);

    fprintf('Average displacement: %.6f   \n', avg_displacement);
    fprintf('Average bond length change: %.6f   \n', avg_bond_change);
    fprintf('Average final bond length: %.6f   \n', avg_final_length);

    % Print bond types and neighbors
    fprintf('Bond types in group:\n');
    for i = 1:length(indices)
        idx = find([h_details.index] == indices(i));
        fprintf('H%d: %s bond to %s(%d)\n', indices(i), ...
            h_details(idx).bond_type, ...
            h_details(idx).neighbor_type, ...
            h_details(idx).neighbor_index);
```

```matlab
    end
end

% [Previous helper functions remain the same]
function [lattice_vectors, atoms] = read_geometry_file(filename)
    % Read the file
    fileID = fopen(filename, 'r');
    if fileID == -1
        error('Could not open file: %s', filename);
    end

    % Initialize variables
    lattice_vectors = zeros(3,3);
    atoms = struct('type', {}, 'coords', {});
    vector_count = 1;

    line = fgetl(fileID);
    while ischar(line)
        % Skip empty lines and comments
        if ~isempty(line) && line(1) ~= '#'
            parts = strsplit(strtrim(line));

            if strcmp(parts{1}, 'lattice_vector')
                lattice_vectors(vector_count,:) = [str2double(parts{2}) str2double(parts{3}) str2double(parts{4})];
                vector_count = vector_count + 1;
            elseif strcmp(parts{1}, 'atom')
                % Skip constraint lines
                if length(parts) >= 5
                    atom_struct = struct();
                    atom_struct.type = parts{5};
                    atom_struct.coords = [str2double(parts{2}) str2double(parts{3}) str2double(parts{4})];
                    atoms = [atoms; atom_struct];
                end
            end
        end
        line = fgetl(fileID);
    end

    fclose(fileID);
end

function cart_coords = frac_to_cart(coords, lattice_vectors)
    % For this case, coordinates are already Cartesian
    cart_coords = coords;
end

function distance = calculate_distance(coord1, coord2, lattice_vectors)
    % Calculate direct distance since coordinates are Cartesian
    diff = coord1 - coord2;
    distance = norm(diff);
end

function [neighbor_indices, distances] = find_nearest_neighbors(atom_idx, atoms, lattice_vectors)
    neighbor_indices = [];
    distances = [];

    for i = 1:length(atoms)
        if i ~= atom_idx
            dist = calculate_distance(atoms(atom_idx).coords, atoms(i).coords, lattice_vectors);
            if dist < 5.0  % Cutoff radius
                neighbor_indices = [neighbor_indices; i];
                distances = [distances; dist];
            end
        end
    end
```

```

    % Sort by distance
    [distances, sort_idx] = sort(distances);
    neighbor_indices = neighbor_indices(sort_idx);
end
```

Listing 2: MATLAB Code to Analyze Thiophene

```
% Main function: analyze_oligothiophene_material.m
function analyze_oligothiophene_material(material_number, oligomer_length)
    % Example usage: analyze_oligothiophene_material(33, 2)

    % Read geometry files
    [lattice_vectors_orig, atoms_orig] = read_geometry_file(['geometry' num2str(material_number) '.in']);
    [lattice_vectors_relaxed, atoms_relaxed] = read_geometry_file(['final_geometry' num2str(material_number) '.in']);

    % Print basic information
    fprintf('\nAnalyzing Material %d (Oligomer Length: %d):\n', material_number, oligomer_length);
    fprintf('Number of atoms read from original file: %d\n', length(atoms_orig));
    fprintf('Number of atoms read from relaxed file: %d\n', length(atoms_relaxed));

    % Analyze hydrogen bonding
    [h_bonds, avg_bond_length, bond_types] = analyze_hydrogen_bonds(atoms_relaxed, lattice_vectors_relaxed);

    % Save results
    results = struct();
    results.h_bonds = h_bonds;
    results.avg_bond_length = avg_bond_length;
    results.bond_types = bond_types;
    results.oligomer_length = oligomer_length;
    save(sprintf('material%d_results.mat', material_number), 'results');

    % Print bond type analysis
    fprintf('\nBond Type Analysis:\n');
    bond_type_names = keys(bond_types);
    for i = 1:length(bond_type_names)
        bond_type = bond_type_names{i};
        bond_lengths = bond_types(bond_type);
        fprintf('%s: Avg Length = %.3f    (Count: %d)\n', ...
            bond_type, mean(bond_lengths), length(bond_lengths));
    end

    fprintf('\nAnalysis complete for Material %d (Oligomer Length: %d).\n', material_number, oligomer_length);
end

% Helper function to analyze hydrogen bonding
function [h_bonds, avg_bond_length, bond_types] = analyze_hydrogen_bonds(atoms, lattice_vectors)
    h_bonds = 0;
    bond_lengths = [];
    bond_types = containers.Map('KeyType', 'char', 'ValueType', 'any');

    for i = 1:length(atoms)
        if strcmp(atoms(i).type, 'H')  % Check only H atoms
            [neighbors, distances] = find_nearest_neighbors(i, atoms, lattice_vectors);

            for j = 1:length(neighbors)
                neighbor_idx = neighbors(j);
                neighbor_type = atoms(neighbor_idx).type;
                bond_type = ['H-' neighbor_type];

                if ~isKey(bond_types, bond_type)
                    bond_types(bond_type) = [];
                end
```

```
                bond_types(bond_type) = [bond_types(bond_type); distances(j)];

                % Count hydrogen bonds (e.g., threshold distance < 2.5    )
                if distances(j) < 2.5
                    h_bonds = h_bonds + 1;
                    bond_lengths = [bond_lengths; distances(j)];
                end
            end
        end
    end

    avg_bond_length = mean(bond_lengths);
end

% Include helper functions (read_geometry_file, find_nearest_neighbors, calculate_distance)
% These should be the same as in your original script.
% Helper function to read geometry files
function [lattice_vectors, atoms] = read_geometry_file(filename)
    fileID = fopen(filename, 'r');
    if fileID == -1
        error('Could not open file: %s', filename);
    end

    lattice_vectors = zeros(3,3);
    atoms = struct('type', {}, 'coords', {});
    vector_count = 1;

    line = fgetl(fileID);
    while ischar(line)
        if ~isempty(line) && line(1) ~= '#'
            parts = strsplit(strtrim(line));
            if strcmp(parts{1}, 'lattice_vector')
                lattice_vectors(vector_count,:) = [str2double(parts{2}) str2double(parts{3}) str2double(parts{4})];
                vector_count = vector_count + 1;
            elseif strcmp(parts{1}, 'atom') && length(parts) >= 5
                atom_struct = struct('type', parts{5}, 'coords', [str2double(parts{2}) str2double(parts{3}) str2double(parts{4})]);
                atoms = [atoms; atom_struct];
            end
        end
        line = fgetl(fileID);
    end

    fclose(fileID);
end

% Helper function to find neighbors
function [neighbor_indices, distances] = find_nearest_neighbors(atom_idx, atoms, lattice_vectors)
    neighbor_indices = [];
    distances = [];
    for i = 1:length(atoms)
        if i ~= atom_idx
            dist = calculate_distance(atoms(atom_idx).coords, atoms(i).coords, lattice_vectors);
            if dist < 5.0
                neighbor_indices = [neighbor_indices; i];
                distances = [distances; dist];
            end
        end
    end
    [distances, sort_idx] = sort(distances);
    neighbor_indices = neighbor_indices(sort_idx);
end

% Helper function to calculate distances
function distance = calculate_distance(coord1, coord2, lattice_vectors)
    diff = coord1 - coord2;
```

```matlab
    distance = norm(diff);
end
```

Listing 3: MATLAB Code to Analyze Oligothiophene

```matlab
function analyze_metal_center_effect()
    materials = struct();

    % Define materials
    materials(1).number = 45;
    materials(1).type = 'Ag/Bi';
    materials(1).metal = 'AgBi';
    materials(1).halide = 'I';

    materials(2).number = 3;
    materials(2).type = 'Pb';
    materials(2).metal = 'Pb';
    materials(2).halide = 'Br';

    % Analyze each material
    for i = 1:length(materials)
        fprintf('\nAnalyzing %s material (Material %d)\n', materials(i).type,
            materials(i).number);
        analyze_single_material(materials(i).number, materials(i).type);
    end

    % Compare and visualize results
    analyze_results(materials);
end

function analyze_results(materials)
    fprintf('\nMetal Center Effect Analysis (Ag/Bi vs Pb)\n');
    fprintf('====================================\n');

    data = struct();
    for i = 1:length(materials)
        filename = sprintf('material%d_results.mat', materials(i).number);
        temp = load(filename);
        data(i).results = temp.results;
    end

    % Generate individual plots
    plot_displacement_comparison(materials, data);
    plot_bond_distribution(materials, data);
    plot_metal_halide_interactions(materials, data);
    plot_displacement_distribution(materials, data);

    % Print detailed statistics
    print_statistics(materials, data);
end

function plot_displacement_comparison(materials, data)
    % Plot Average Displacement Comparison
    avg_disp = zeros(1, length(data));
    std_disp = zeros(1, length(data));

    for i = 1:length(data)
        avg_disp(i) = mean(data(i).results.displacements);
        std_disp(i) = std(data(i).results.displacements);
    end

    figure;
    bar(avg_disp, 'FaceColor', [0.2 0.6 0.8]);
    hold on;
    errorbar(1:length(data), avg_disp, std_disp, 'k.', 'LineWidth', 1.5);
    hold off;

    set(gca, 'XTickLabel', {materials.type}, 'FontSize', 12);
    title('Average H Displacement', 'FontSize', 14, 'FontWeight', 'bold');
```

```
    ylabel('Displacement (  )', 'FontSize', 12);
    saveas(gcf, 'avg_displacement_comparison.png');
end

function plot_bond_distribution(materials, data)
    % Plot Bond Type Distribution
    all_types = {};
    for i = 1:length(data)
        all_types = union(all_types, keys(data(i).results.bond_types));
    end

    counts = zeros(length(data), length(all_types));
    for i = 1:length(data)
        for j = 1:length(all_types)
            if isKey(data(i).results.bond_types, all_types{j})
                counts(i, j) = length(data(i).results.bond_types(all_types{j}));
            end
        end
    end

    figure;
    bar(counts, 'stacked');
    colormap(lines(length(all_types))); % Ensure distinct colors for each bond type
    legend(all_types, 'Location', 'northeastoutside', 'FontSize', 10);
    set(gca, 'XTickLabel', {materials.type}, 'FontSize', 12);
    title('Bond Type Distribution', 'FontSize', 14, 'FontWeight', 'bold');
    ylabel('Count', 'FontSize', 12);
    xlabel('Material Type', 'FontSize', 12);
    saveas(gcf, 'bond_type_distribution.png');
end

function plot_metal_halide_interactions(materials, data)
    % Plot Metal and Halide Interactions
    metal_interactions = zeros(2, length(materials));

    for i = 1:length(data)
        metal_bond = ['H-' materials(i).metal];
        halide_bond = ['H-' materials(i).halide];

        if isKey(data(i).results.bond_types, metal_bond)
            metal_interactions(1, i) = mean(data(i).results.bond_types(metal_bond));
        end
        if isKey(data(i).results.bond_types, halide_bond)
            metal_interactions(2, i) = mean(data(i).results.bond_types(halide_bond));
        end
    end

    figure;
    bar(metal_interactions', 'grouped');
    set(gca, 'XTickLabel', {materials.type}, 'FontSize', 12);
    legend('Metal-H', 'Halide-H', 'Location', 'best', 'FontSize', 12);
    title('Metal and Halide Interactions', 'FontSize', 14, 'FontWeight', 'bold');
    ylabel('Average Distance (  )', 'FontSize', 12);
    saveas(gcf, 'metal_halide_interactions.png');
end

function plot_displacement_distribution(materials, data)
    % Plot Displacement Distribution
    figure;
    hold on;
    colors = lines(length(materials));
    for i = 1:length(data)
        histogram(data(i).results.displacements, 'DisplayName', materials(i).type, ...
            'FaceColor', colors(i, :), 'FaceAlpha', 0.5, 'BinWidth', 0.02);
    end
    hold off;

    legend('Location', 'northeastoutside', 'FontSize', 12);
    title('H Displacement Distribution', 'FontSize', 14, 'FontWeight', 'bold');
```

```
    xlabel('Displacement (  )', 'FontSize', 12);
    ylabel('Frequency', 'FontSize', 12);
    saveas(gcf, 'displacement_distribution.png');
end

function print_statistics(materials, data)
    fprintf('\nDetailed Comparison:\n');

    for i = 1:length(materials)
        fprintf('\n%s Material Analysis:\n', materials(i).type);
        fprintf('Average displacement: %.6f    %.6f   \n', ...
            mean(data(i).results.displacements), ...
            std(data(i).results.displacements));

        fprintf('Bond Types:\n');
        types = keys(data(i).results.bond_types);
        for j = 1:length(types)
            bond_type = types{j};
            lengths = data(i).results.bond_types(bond_type);
            fprintf('  %s: %.3f    %.3f    (Count: %d)\n', ...
                bond_type, mean(lengths), std(lengths), length(lengths));
        end
    end
end
```

Listing 4: MATLAB Code to Analyze Metal Centres

```
function analyze_polycyclic_aromatic_systems()
    materials = struct();

    % Define materials
    materials(1).number = 7;
    materials(1).type = 'Naphthyl-System-1';
    materials(1).ring = 'Naphthyl';

    materials(2).number = 27;
    materials(2).type = 'Naphthyl-System-2';
    materials(2).ring = 'Naphthyl';

    materials(3).number = 25;
    materials(3).type = 'Anthryl-System-1';
    materials(3).ring = 'Anthryl';

    materials(4).number = 26;
    materials(4).type = 'Anthryl-System-2';
    materials(4).ring = 'Anthryl';

    % Analyze individual materials
    for i = 1:length(materials)
        fprintf('\nAnalyzing %s (Material %d)\n', materials(i).type, materials(i).number);
        analyze_single_material(materials(i).number, materials(i).type);
    end

    % Perform comparison and visualization
    analyze_results(materials);
end

function analyze_results(materials)
    fprintf('\nComparison of Polycyclic Aromatic Systems\n');
    fprintf('=======================================\n');

    data = struct();
    for i = 1:length(materials)
        filename = sprintf('material%d_results.mat', materials(i).number);
        temp = load(filename);
        data(i).results = temp.results;
    end

    % Generate visualizations
```

```
    plot_displacement_by_ring(materials, data);
    plot_bond_distribution_by_ring(materials, data);
    plot_average_bond_length(materials, data);
    plot_maximum_displacement(materials, data);

    % Print detailed statistics
    print_statistics(materials, data);
end

function plot_displacement_by_ring(materials, data)
    % Average Displacement by Ring System
    rings = unique({materials.ring});
    avg_displacement = zeros(1, length(rings));
    std_displacement = zeros(1, length(rings));

    for r = 1:length(rings)
        ring_indices = find(strcmp({materials.ring}, rings{r}));
        displacements = [];
        for i = ring_indices
            displacements = [displacements; data(i).results.displacements];
        end
        avg_displacement(r) = mean(displacements);
        std_displacement(r) = std(displacements);
    end

    figure;
    bar(avg_displacement);
    hold on;
    errorbar(1:length(rings), avg_displacement, std_displacement, 'k.', 'LineWidth', 1.5);
    hold off;

    set(gca, 'XTickLabel', rings, 'FontSize', 12);
    ylabel('Average Displacement (  )', 'FontSize', 12);
    title('Average Displacement by Aromatic Ring System', 'FontSize', 12, 'FontWeight',
        'bold');
    saveas(gcf, 'displacement_by_ring.png');
end

function plot_bond_distribution_by_ring(materials, data)
    % Bond Type Distribution for Each Ring System
    rings = unique({materials.ring});
    all_bond_types = {};
    for i = 1:length(data)
        all_bond_types = union(all_bond_types, keys(data(i).results.bond_types));
    end

    bond_counts = zeros(length(rings), length(all_bond_types));
    for r = 1:length(rings)
        ring_indices = find(strcmp({materials.ring}, rings{r}));
        for i = ring_indices
            for j = 1:length(all_bond_types)
                if isKey(data(i).results.bond_types, all_bond_types{j})
                    bond_counts(r, j) = bond_counts(r, j) +
                        length(data(i).results.bond_types(all_bond_types{j}));
                end
            end
        end
    end

    figure;
    bar(bond_counts, 'stacked');
    colormap(lines(length(all_bond_types))); % Distinct colors
    legend(all_bond_types, 'Location', 'northeastoutside', 'FontSize', 10);
    set(gca, 'XTickLabel', rings, 'FontSize', 12);
    ylabel('Count', 'FontSize', 12);
    title('Bond Type Distribution by Ring System', 'FontSize', 12, 'FontWeight', 'bold');
    saveas(gcf, 'bond_distribution_by_ring.png');
end

```

```
function plot_average_bond_length(materials, data)
    % Average Bond Length by Ring System
    rings = unique({materials.ring});
    avg_bond_lengths = zeros(1, length(rings));

    for r = 1:length(rings)
        ring_indices = find(strcmp({materials.ring}, rings{r}));
        bond_lengths = [];
        for i = ring_indices
            bond_lengths = [bond_lengths; data(i).results.final_bond_lengths];
        end
        avg_bond_lengths(r) = mean(bond_lengths);
    end

    figure;
    bar(avg_bond_lengths, 'FaceColor', [0.6 0.8 0.6]);
    set(gca, 'XTickLabel', rings, 'FontSize', 12);
    ylabel('Average Bond Length (  )', 'FontSize', 12);
    title('Average Bond Length by Aromatic Ring System', 'FontSize', 12, 'FontWeight', 'bold');
    saveas(gcf, 'average_bond_length_by_ring.png');
end

function plot_maximum_displacement(materials, data)
    % Maximum Displacement by Ring System
    rings = unique({materials.ring});
    max_displacement = zeros(1, length(rings));

    for r = 1:length(rings)
        ring_indices = find(strcmp({materials.ring}, rings{r}));
        max_disp = [];
        for i = ring_indices
            max_disp = [max_disp; max(data(i).results.displacements)];
        end
        max_displacement(r) = max(max_disp);
    end

    figure;
    bar(max_displacement, 'FaceColor', [0.8 0.6 0.6]);
    set(gca, 'XTickLabel', rings, 'FontSize', 12);
    ylabel('Maximum Displacement (  )', 'FontSize', 12);
    title('Maximum Displacement by Aromatic Ring System', 'FontSize', 12, 'FontWeight', 'bold');
    saveas(gcf, 'maximum_displacement_by_ring.png');
end

function print_statistics(materials, data)
    fprintf('\nDetailed Statistics for Polycyclic Aromatic Systems:\n');
    fprintf('---------------------------------------------------\n');

    rings = unique({materials.ring});
    for r = 1:length(rings)
        fprintf('\n%s:\n', rings{r});
        ring_indices = find(strcmp({materials.ring}, rings{r}));
        displacements = [];
        bond_lengths = [];

        for i = ring_indices
            displacements = [displacements; data(i).results.displacements];
            bond_lengths = [bond_lengths; data(i).results.final_bond_lengths];
        end

        fprintf('  Average Displacement: %.6f    %.6f   \n', mean(displacements), std(displacements));
        fprintf('  Average Bond Length: %.6f    %.6f   \n', mean(bond_lengths), std(bond_lengths));
    end
end
```

Listing 5: MATLAB Code to Analyze Aromatic

```
function analyze_phenyl_based_systems()
    materials = struct();

    % Define materials
    materials(1).number = 11;
    materials(1).type = 'Phenyl-Br';
    materials(1).group = 'Halide';

    materials(2).number = 12;
    materials(2).type = 'Phenyl-Cl';
    materials(2).group = 'Halide';

    materials(3).number = 13;
    materials(3).type = 'Phenyl-I';
    materials(3).group = 'Halide';

    materials(4).number = 80;
    materials(4).type = 'Phenyl-F';
    materials(4).group = 'Fluorine';

    materials(5).number = 107;
    materials(5).type = 'Phenyl-Dimethyl-1';
    materials(5).group = 'Dimethyl';

    materials(6).number = 108;
    materials(6).type = 'Phenyl-Dimethyl-2';
    materials(6).group = 'Dimethyl';

    % Analyze individual materials
    for i = 1:length(materials)
        fprintf('\nAnalyzing %s (Material %d)\n', materials(i).type, materials(i).number);
        analyze_single_material(materials(i).number, materials(i).type);
    end

    % Perform comparative analysis
    analyze_results(materials);
end

function analyze_results(materials)
    fprintf('\nComparative Analysis of Phenyl-Based Systems\n');
    fprintf('===========================================\n');

    data = struct();
    for i = 1:length(materials)
        filename = sprintf('material%d_results.mat', materials(i).number);
        temp = load(filename);
        data(i).results = temp.results;
    end

    % Generate visualizations
    plot_displacement_by_group(materials, data);
    plot_bond_distribution_by_group(materials, data);
    plot_average_bond_length(materials, data);
    plot_maximum_displacement(materials, data);

    % Print detailed statistics
    print_statistics(materials, data);
end

function plot_displacement_by_group(materials, data)
    % Average Displacement by Group
    groups = unique({materials.group});
    avg_displacement = zeros(1, length(groups));
    std_displacement = zeros(1, length(groups));

    for g = 1:length(groups)
        group_indices = find(strcmp({materials.group}, groups{g}));
        displacements = [];
        for i = group_indices
```

```
            displacements = [displacements; data(i).results.displacements];
        end
        avg_displacement(g) = mean(displacements);
        std_displacement(g) = std(displacements);
    end

    figure;
    bar(avg_displacement);
    hold on;
    errorbar(1:length(groups), avg_displacement, std_displacement, 'k.', 'LineWidth', 1.5);
    hold off;

    set(gca, 'XTickLabel', groups, 'FontSize', 12);
    ylabel('Average Displacement (  )', 'FontSize', 12);
    title('Average Displacement by Phenyl Group', 'FontSize', 14, 'FontWeight', 'bold');
    saveas(gcf, 'displacement_by_group.png');
end

function plot_bond_distribution_by_group(materials, data)
    % Bond Type Distribution for Each Group
    groups = unique({materials.group});
    all_bond_types = {};
    for i = 1:length(data)
        all_bond_types = union(all_bond_types, keys(data(i).results.bond_types));
    end

    bond_counts = zeros(length(groups), length(all_bond_types));
    for g = 1:length(groups)
        group_indices = find(strcmp({materials.group}, groups{g}));
        for i = group_indices
            for j = 1:length(all_bond_types)
                if isKey(data(i).results.bond_types, all_bond_types{j})
                    bond_counts(g, j) = bond_counts(g, j) +
                        length(data(i).results.bond_types(all_bond_types{j}));
                end
            end
        end
    end

    figure;
    bar(bond_counts, 'stacked');
    colormap(lines(length(all_bond_types))); % Distinct colors
    legend(all_bond_types, 'Location', 'northeastoutside', 'FontSize', 10);
    set(gca, 'XTickLabel', groups, 'FontSize', 12);
    ylabel('Count', 'FontSize', 12);
    title('Bond Type Distribution by Phenyl Group', 'FontSize', 14, 'FontWeight', 'bold');
    saveas(gcf, 'bond_distribution_by_group.png');
end

function plot_average_bond_length(materials, data)
    % Average Bond Length by Group
    groups = unique({materials.group});
    avg_bond_lengths = zeros(1, length(groups));

    for g = 1:length(groups)
        group_indices = find(strcmp({materials.group}, groups{g}));
        bond_lengths = [];
        for i = group_indices
            bond_lengths = [bond_lengths; data(i).results.final_bond_lengths];
        end
        avg_bond_lengths(g) = mean(bond_lengths);
    end

    figure;
    bar(avg_bond_lengths, 'FaceColor', [0.6 0.8 0.6]);
    set(gca, 'XTickLabel', groups, 'FontSize', 12);
    ylabel('Average Bond Length (  )', 'FontSize', 12);
    title('Average Bond Length by Phenyl Group', 'FontSize', 14, 'FontWeight', 'bold');
    saveas(gcf, 'average_bond_length_by_group.png');
```

```matlab
end

function plot_maximum_displacement(materials, data)
    % Maximum Displacement by Group
    groups = unique({materials.group});
    max_displacement = nan(1, length(groups)); % Initialize with NaN to handle empty groups

    for g = 1:length(groups)
        group_indices = find(strcmp({materials.group}, groups{g}));
        max_disp = [];
        for i = group_indices
            if ~isempty(data(i).results.displacements)
                max_disp = [max_disp; max(data(i).results.displacements)];
            end
        end
        if ~isempty(max_disp) % Check if the group has valid displacements
            max_displacement(g) = max(max_disp);
        else
            max_displacement(g) = NaN; % Assign NaN if no data is available
        end
    end

    figure;
    bar(max_displacement, 'FaceColor', [0.8 0.6 0.6]);
    set(gca, 'XTickLabel', groups, 'FontSize', 12);
    ylabel('Maximum Displacement (  )', 'FontSize', 12);
    title('Maximum Displacement by Phenyl Group', 'FontSize', 14, 'FontWeight', 'bold');
    saveas(gcf, 'maximum_displacement_by_group.png');
end

function print_statistics(materials, data)
    fprintf('\nDetailed Statistics:\n');
    groups = unique({materials.group});
    for g = 1:length(groups)
        fprintf('\nGroup: %s\n', groups{g});
        group_indices = find(strcmp({materials.group}, groups{g}));
        for i = group_indices
            fprintf('  %s:\n', materials(i).type);
            fprintf('    Average displacement: %.6f    %.6f   \n', ...
                mean(data(i).results.displacements), ...
                std(data(i).results.displacements));
            fprintf('    Average bond length: %.6f    %.6f   \n', ...
                mean(data(i).results.final_bond_lengths), ...
                std(data(i).results.final_bond_lengths));
        end
    end
end
```

Listing 6: MATLAB Code to Analyze Phenyl

```matlab
function analyze_aliphatic_systems()
    materials = struct();

    % Define materials for aliphatic systems
    materials(1).number = 97;
    materials(1).type = 'Aliphatic-System-1';
    materials(1).group = 'Aliphatic';

    materials(2).number = 114;
    materials(2).type = 'Aliphatic-System-2';
    materials(2).group = 'Aliphatic';

    % Define materials for aromatic comparison
    materials(3).number = 7; % Naphthyl
    materials(3).type = 'Aromatic-Naphthyl';
    materials(3).group = 'Aromatic';

    materials(4).number = 25; % Anthryl
    materials(4).type = 'Aromatic-Anthryl';
```

```
    materials(4).group = 'Aromatic';

    % Analyze each material
    for i = 1:length(materials)
        fprintf('\nAnalyzing %s (Material %d)\n', materials(i).type, materials(i).number);
        analyze_single_material(materials(i).number, materials(i).type);
    end

    % Process results and generate comparisons
    analyze_results(materials);
end

function analyze_results(materials)
    fprintf('\nComparative Analysis of Aliphatic and Aromatic Systems\n');
    fprintf('=====================================================\n');

    data = struct();
    for i = 1:length(materials)
        filename = sprintf('material%d_results.mat', materials(i).number);
        temp = load(filename);
        data(i).results = temp.results;
    end

    % Generate individual plots
    plot_average_displacement(materials, data);
    plot_bond_length_distribution(materials, data);
    plot_bond_type_comparison(materials, data);

    % Print statistics
    print_statistics(materials, data);
end

function plot_average_displacement(materials, data)
    % Calculate average displacement for each material
    groups = unique({materials.group});
    avg_disp = zeros(1, length(groups));
    std_disp = zeros(1, length(groups));

    for g = 1:length(groups)
        group_indices = find(strcmp({materials.group}, groups{g}));
        group_displacements = [];
        for i = group_indices
            group_displacements = [group_displacements; data(i).results.displacements];
        end
        avg_disp(g) = mean(group_displacements);
        std_disp(g) = std(group_displacements);
    end

    % Create the plot
    figure;
    bar(avg_disp);
    hold on;
    errorbar(1:length(groups), avg_disp, std_disp, 'k.', 'LineWidth', 1.5);
    hold off;
    set(gca, 'XTickLabel', groups);
    ylabel('Average Displacement (  )');
    title('Average H Displacement: Aliphatic vs Aromatic');
    saveas(gcf, 'average_displacement_aliphatic_aromatic.png');
end

function plot_bond_length_distribution(materials, data)
    % Collect bond length data for aliphatic and aromatic groups
    groups = unique({materials.group});
    group_bond_lengths = cell(1, length(groups));

    for g = 1:length(groups)
        group_indices = find(strcmp({materials.group}, groups{g}));
        bond_lengths = [];
        for i = group_indices
```

```
            bond_lengths = [bond_lengths; data(i).results.final_bond_lengths];
        end
        group_bond_lengths{g} = bond_lengths;
    end

    % Create boxplot
    figure;
    boxplot(vertcat(group_bond_lengths{:}), ...
            repelem(1:length(groups), cellfun(@length, group_bond_lengths)), ...
            'Labels', groups);
    ylabel('Bond Length (  )');
    title('Bond Length Distribution: Aliphatic vs Aromatic');
    saveas(gcf, 'bond_length_distribution_aliphatic_aromatic.png');
end

function plot_bond_type_comparison(materials, data)
    % Gather bond type counts for each group
    groups = unique({materials.group});
    all_types = {};
    for i = 1:length(data)
        all_types = union(all_types, keys(data(i).results.bond_types));
    end

    counts = zeros(length(groups), length(all_types));
    for g = 1:length(groups)
        group_indices = find(strcmp({materials.group}, groups{g}));
        for t = 1:length(all_types)
            bond_type = all_types{t};
            for i = group_indices
                if isKey(data(i).results.bond_types, bond_type)
                    counts(g, t) = counts(g, t) +
                        length(data(i).results.bond_types(bond_type));
                end
            end
        end
    end

    % Create bar chart
    figure;
    bar(counts, 'stacked');
    legend(all_types, 'Location', 'best');
    set(gca, 'XTickLabel', groups);
    ylabel('Count');
    title('Bond Type Distribution: Aliphatic vs Aromatic');
    saveas(gcf, 'bond_type_comparison_aliphatic_aromatic.png');
end

function print_statistics(materials, data)
    fprintf('\nDetailed Statistics:\n');
    groups = unique({materials.group});

    for g = 1:length(groups)
        fprintf('\nGroup: %s\n', groups{g});
        group_indices = find(strcmp({materials.group}, groups{g}));

        for i = group_indices
            fprintf('  %s:\n', materials(i).type);
            fprintf('    Average displacement: %.6f    %.6f   \n', ...
                mean(data(i).results.displacements), ...
                std(data(i).results.displacements));
            fprintf('    Average bond length: %.6f    %.6f   \n', ...
                mean(data(i).results.final_bond_lengths), ...
                std(data(i).results.final_bond_lengths));
        end
    end
end
```

Listing 7: MATLAB Code to Analyze Aliphatic

```matlab
function analyze_cross_group()
    materials = struct();

    % Define materials
    materials(1).number = 3; % Br
    materials(1).type = 'Quaterthiophene-Br';
    materials(1).group = 'Halide';
    materials(1).halide = 'Br';

    materials(2).number = 21; % Cl
    materials(2).type = 'Quaterthiophene-Cl';
    materials(2).group = 'Halide';
    materials(2).halide = 'Cl';

    materials(3).number = 22; % I
    materials(3).type = 'Quaterthiophene-I';
    materials(3).group = 'Halide';
    materials(3).halide = 'I';

    materials(4).number = 80; % Fluorinated system
    materials(4).type = 'Phenyl-F';
    materials(4).group = 'Cation';
    materials(4).cation = 'Fluorinated';

    materials(5).number = 107; % Dimethyl-1
    materials(5).type = 'Phenyl-Dimethyl-1';
    materials(5).group = 'Cation';
    materials(5).cation = 'Dimethyl';

    materials(6).number = 108; % Dimethyl-2
    materials(6).type = 'Phenyl-Dimethyl-2';
    materials(6).group = 'Cation';
    materials(6).cation = 'Dimethyl';

    % Analyze each material
    for i = 1:length(materials)
        fprintf('\nAnalyzing %s (Material %d)\n', materials(i).type, materials(i).number);
        analyze_single_material(materials(i).number, materials(i).type);
    end

    % Process results and generate comparisons
    analyze_results(materials);
end

function analyze_results(materials)
    fprintf('\nCross-Group Analysis\n');
    fprintf('=====================\n');

    data = struct();
    for i = 1:length(materials)
        filename = sprintf('material%d_results.mat', materials(i).number);
        temp = load(filename);
        data(i).results = temp.results;
    end

    % Generate individual plots
    plot_halide_effects(materials, data);
    plot_cation_structure_property(materials, data);

    % Print detailed statistics
    print_statistics(materials, data);
end

function plot_halide_effects(materials, data)
    % Filter materials by halides
    halides = {'Br', 'Cl', 'I'};
    material_halides = arrayfun(@(m) convertToString(m.halide), materials, 'UniformOutput',
        false);
    halide_indices = find(cellfun(@(x) ismember(x, halides), material_halides));
```

```matlab

    avg_disp = zeros(1, length(halides));
    avg_bond_lengths = zeros(1, length(halides));

    for h = 1:length(halides)
        idx = halide_indices(strcmp(material_halides(halide_indices), halides{h}));
        if ~isempty(idx)
            avg_disp(h) = mean(data(idx).results.displacements);
            avg_bond_lengths(h) = mean(data(idx).results.final_bond_lengths);
        end
    end

    % Plot displacement and bond lengths
    figure;
    subplot(2, 1, 1);
    bar(avg_disp);
    set(gca, 'XTickLabel', halides);
    ylabel('Average Displacement (  )');
    title('Halide Effects: Displacement');

    subplot(2, 1, 2);
    bar(avg_bond_lengths);
    set(gca, 'XTickLabel', halides);
    ylabel('Average Bond Length (  )');
    title('Halide Effects: Bond Length');

    saveas(gcf, 'halide_effects.png');
end

function plot_cation_structure_property(materials, data)
    % Ensure `materials.cation` is consistently stringified
    cation_names = arrayfun(@(m) convertToString(m.cation), materials, 'UniformOutput', false);
    cations = unique(cation_names);

    avg_disp = zeros(1, length(cations));
    avg_bond_lengths = zeros(1, length(cations));

    for c = 1:length(cations)
        cation_indices = find(strcmp(cation_names, cations{c}));
        cation_displacements = [];
        cation_bond_lengths = [];

        for i = cation_indices
            cation_displacements = [cation_displacements; data(i).results.displacements];
            cation_bond_lengths = [cation_bond_lengths; data(i).results.final_bond_lengths];
        end

        avg_disp(c) = mean(cation_displacements);
        avg_bond_lengths(c) = mean(cation_bond_lengths);
    end

    % Create scatter plot for structure-property relationships
    figure;
    scatter(avg_disp, avg_bond_lengths, 50, 'filled');
    text(avg_disp, avg_bond_lengths, cations, 'VerticalAlignment', 'bottom', 'HorizontalAlignment', 'right');
    xlabel('Average Displacement (  )');
    ylabel('Average Bond Length (  )');
    title('Structure-Property Relationships');
    saveas(gcf, 'structure_property_relationships.png');
end

function print_statistics(materials, data)
    fprintf('\nDetailed Analysis:\n');
    fprintf('=================\n');

    groups = unique({materials.group});
    for g = 1:length(groups)
```

```
        fprintf('\nGroup: %s\n', groups{g});
        group_indices = find(strcmp({materials.group}, groups{g}));

        for i = group_indices
            fprintf('  %s:\n', materials(i).type);
            fprintf('    Average displacement: %.6f    %.6f   \n', ...
                mean(data(i).results.displacements), ...
                std(data(i).results.displacements));
            fprintf('    Average bond length: %.6f    %.6f   \n', ...
                mean(data(i).results.final_bond_lengths), ...
                std(data(i).results.final_bond_lengths));
        end
    end
end

function str = convertToString(input)
    if ischar(input) || isstring(input)
        str = char(input);
    elseif isnumeric(input)
        str = num2str(input);
    else
        str = '';
    end
end
```

Listing 8: MATLAB Code to Analyze Cross Materials