Modeling Biphenylene Network (BPN) with SNAP-Based Machine Learning Potential

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This research focuses on the development and validation of machine learning interatomic potentials (MLIAPs) for the biphenylene network (BPN) [1], using the Spectral Neighbor Analysis Potential (SNAP) [2] framework. BPN, a two-dimensional carbon allotrope, demonstrates metallic conductivity and a unique periodic arrangement of sp^2-hybridized carbon atoms. SNAP is utilized to accurately model the complex bonding interactions within BPN, reducing computational costs while maintaining high fidelity in comparison to density functional theory (DFT) calculations. Training datasets are generated through DFT simulations, which include various strained and displaced atom configurations, while keeping the cell vectors of BPN unchanged. Validation tests confirm the robustness of SNAP in predicting energies and forces. Furthermore, the thermal conductivity of BPN is computed using molecular dynamics simulations based on the Green-Kubo [3][4][5] method, implemented in LAMMPS, with results showing excellent agreement with DFT-based calculations. This study provides a pathway for efficient simulations of BPN, which could be valuable for potential applications in electronics and materials science.

References

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