Introduction

The present project investigates the molecular dynamics (MD) simulations of perovskite-based materials, specifically focusing on their potential for solar energy conversion to electrical energy. Perovskite materials, notably methylammonium lead iodide (MAPbI3), have emerged as promising candidates in the realm of photovoltaics due to their advantageous optoelectronic properties, including high absorption coefficients, tunable band gaps, and exceptional charge transport characteristics. This study aims to utilize LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) to model the atomic-level interactions and dynamics within these materials under various thermal and mechanical conditions.

The MD simulations are designed to analyze the structural stability, thermodynamic properties, and charge transport mechanisms in MAPbI3 under different environmental stimuli. By employing a hybrid potential approach that incorporates both pairwise additive potentials and long-range electrostatics, we aim to accurately replicate the interactions governing the material's behavior. Furthermore, the project leverages advanced computational techniques to extract thermodynamic data, enabling a comprehensive understanding of the material's phase transitions and energy conversion efficiencies.

Key parameters such as temperature, pressure, and volume will be systematically varied, allowing for an in-depth analysis of the perovskite structure's response to external forces. The output of the simulations will be scrutinized through thermodynamic ensemble averages and radial distribution functions, providing insights into the molecular organization and dynamics at play. Ultimately, this project seeks to contribute to the ongoing research in energy harvesting technologies by elucidating the fundamental mechanisms that dictate the performance of perovskite-based solar cells.