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ABSTRACT SYMPOSIUM NAME: Solid-State Inorganic Chemistry

ABSTRACT SYMPOSIUM PROGRAM AREA NAME: INOR

CONTROL ID: 3553733

PRESENTATION TYPE: Oral Only : Do not consider for Sci-Mix

TITLE: Development and validation of ReaxFF forcefield for solid-state ion conduction in Ag/S-based systems

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ABSTRACT BODY:

Abstract: Solid-state ion conduction (SSIC) is a mechanism of ionic current that has garnered increasing attention for applications in all-solid-state batteries and atomic switches. The Ag/S SSIC system in β -Ag₂S, possessing the highest ionic conductivity of any known material, provides a unique opportunity to better understand the fundamental nature of SSIC. β -Ag₂S is topographically similar to binary perovskites except that it is cubic, leading to isotropic SSIC exceeding 4 S/cm. The dynamic nature of SSIC makes it difficult to study by observational means, where inherent time-averaging obscures correlations among atomic transit routes. Molecular dynamics (MD) is a tool ideally suited for gaining insight into large atomic systems with sub-nanosecond time resolutions. However, traditional MD potentials lack a description of bond-breaking/forming reactions, which are an essential aspect of SSIC and related memristic properties. This limitation can be overcome by using a reactive force field (ReaxFF), which enables the simulation of bonding reactions with DFT-level accuracy.

In this study, we present a ReaxFF force field for the Ag/S system, optimized for simulating SSIC in β -Ag₂S. Training data consisted of crystal structures, Bader partial charges, and energies of various Ag/S clusters calculated at the DFT-level. Energies were obtained with Gaussian 16, using the PBEh1PBE hybrid functional with a triple-zeta correlation-consistent basis set. Multiobjective parameter optimization was accomplished with an updated form of the Genetic Algorithm for Reactive Force Fields (GARFField). The force field was validated with potential energy and ion conductivity calculations, along with relevant structural features. Results were compared with equivalent simulations from other established potentials. This new ReaxFF force field will enable modeling of realistic SSIC configurations for Ag/S-based materials and provides a viable approach for extending ReaxFF to other SSIC systems in the future. This work was supported by the National Science Foundation under grant #2025319.

(No Image Selected)

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Product version number 4.17.3 (Build 37). Build date Fri Jan 15 10:20:49 EST 2021. Server ip-10-236-28-131