Abstract Submitted
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Environment Dependent Dynamic Charge Interatomic Potential for Silica LEX KEMPER, KRISHNA MURALIDHARAN, YINGXIA WAN, HAI-PING CHENG, University of Florida — We present a new interatomic potential to model the various silica polymorphs. Our formulation is loosely based on the embedded atom method (EAM), and accounts for explicit charge variations of atoms as a function of the local chemical environment of atoms. The parameters for the potential are derived from density functional (DFT) calculations. Some preliminary results will be discussed. Work supported by NSF ITR award DMR-0325553.

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