Abstract Submitted
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Ab initio molecular dynamics simulations of molten $Al_{1-x}Si_x$ alloys[1] M. KIM, K. H. KHOO, University of Texas at Austin, T.-L. CHAN, Resselaer Polytechnic Institute, G. SCHOFIELD, JAMES R. CHELIKOWSKY, University of Texas at Austin — First-principles molecular dynamics simulations have been performed to study the structure and dynamics of molten $Al_{1-x}Si_x$ alloys over a range of alloy compositions and temperatures. Employing an efficient real-space density functional method coupled with a subspace filtering algorithm, we were able to perform simulations on large systems by avoiding explicit eigenvalue calculations. The calculated static structure factors show excellent agreement with data from X-ray diffraction experiments. The composition and temperature dependence of the simulated microstructure and atomic diffusivity will also be discussed.

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