Abstract Submitted
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Prospects for efficient QMC defect calculations: the energy density applied to Ge self-interstitials[1] JARON KROGEL, University of Illinois at Urbana-Champaign, JEONGNIM KIM, Oak Ridge National Laboratory, DAVID CEPERLEY, University of Illinois at Urbana-Champaign — Defect formation energies require expensive energy difference calculations between defective and bulk systems over a range of system sizes. At the point of convergence, subregions added to represent larger systems no longer contribute to the formation energy and therefore display similar local energetics. A recent formulation of the energy density for QMC is capable of identifying separate energetic contributions from each atom, enabling the identification of the bulk-like regions in a defect system that only add noise to the final result. The potential efficiency gains of this approach are explored in a realistic defect system, the germanium self-interstitial. Calculations involving up to 217 atoms at fixed volume show that the extent of the strain energy field depends strongly on the interstitial site. Bulk-like regions are largest for the hexagonal interstitial increasing the efficiency by a factor of 2-3. In contrast, the split structure interstitial has few bulk-like atoms and shows no speedup. Possible approaches to further improve the efficiency will be discussed.

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