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Atomistic Simulation as a Predictive Tool: The Case of Gallium

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In this talk we will discuss the predictive capabilities of atomistic simulation based on classical semi-empirical potentials and density-functional theory (DFT) calculation. As a specific example, we consider the properties of the condensed phases of the element Gallium (Ga). Using DFT and modified-embedded-atom-model (MEAM) calculations we predict the existence of a novel metastable crystalline phase of elemental Ga as well as the occurrence a first-order liquid-liquid phase transition in the metastable supercooled liquid phase.
The prediction of the existence of an unknown metastable crystalline phase of Gallium is obtained by the combination of MEAM-based molecular dynamics (MD) simulations and DFT calculations. The MD simulations reveal the unknown crystalline form through a first-order phase transition originating from the *Cmca* symmetric A11-Ga phase under hydrostatic tension. Subsequently, the DFT calculations using two different exchange-correlation functionals are employed to verify its stability and determine its electronic structure. The structure of the orthorhombic phase is described by symmetry group *Cmcm* and shows a dimer arrangement resembling of the A11-Ga phase. A first-order phase transition from A11-Ga to the unknown phase is estimated to occur at -1.3 GPa.
In addition we present theoretical results that lend support to recent experimental observations suggesting the existence of a first-order liquid-liquid phase transformation (LLPT) in Gallium. Using MEAM-based MD simulations we observe a transition from a high-density to a low-density liquid in the supercooled regime. The first-order character of the transition is established through the detection of the release of latent heat and our findings suggest that the LLPT terminates in a critical point that is located in the tensile-strained domain of the metastable phase diagram.