Towards a General-Purpose Interatomic Potential for Silicon Carbide

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SiC is a prototypical material for high temperature applications (e.g aerospace, automotive and thermoelectric) involving complex microscopic processes typically inaccessible to experiments [1]. To gain insight into the functional properties of e.g. SiC nanostructures, computationally expensive quantum mechanical methods such as density functional theory (DFT) must be employed. This is because less computationally demanding methods are almost always not accurate enough. In fact, similar to Si and C alone, various empirical interatomic potentials have been developed for SiC, such as Tersoff or Stillinger-Weber [2,3]. These potentials are designed to reproduce specific features of the material, at the expense of transferability to a wider range of functional properties. The aim of this project is to build a general purpose interatomic potential for SiC (e.g using machine-learning regression starting from a DFT dataset of representative configurations [4,5]). As a first step towards achieving this goal we here report a comparative study of the performance of currently available models for SiC [2,3,6], focussing in particular on the structural properties of the liquid phase.

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