Si many-body potentials: the state of the art and beyond

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Empirical potential development is a two-step process: a physically sound functional form is proposed and then the parameters of the potential function are obtained. There have been many potential forms proposed for the last three decades, but none of them are entirely successful in predicting the mechanical properties of bulk silicon. We have found that even a reasonably good functional form can fail to reproduce the equilibrium bulk properties all because of the fitting process, leading to a premature conclusion that the functional form is not correctly derived.
In this talk, the famous Tersoff potential is rediscovered in terms of the fitting process. In particular, the systematic determination of potential parameters are discussed and compared with the conventional fitting process. The reproducibility of the input database and the transferability outside the input database are discussed. We try to rigorously identify the potentials and limitations of Tersoff potentials.

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