MULTI−CONFIGURATION SAMPLING FOR MODELLING CARBONATE SOLID SOLUTIONS

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Conventional defect calculations using periodic systems with point defects are restricted to the dilute limit and have therefore struggled to model successfully solid solutions and highly disordered solids. These systems need to be modelled by sampling and averaging the range of configurations available. We demonstrate how Lattice Dynamics and Monte Carlo methods can be modified to take account of the multiple configurations needed to model a highly non−ideal solid system.

Carbonate solid systems, specifically dolomite ($CaMg(CO_3)_2$), have proved exceptionally difficult to study experimentally making them an engaging system for computational modelling. We have applied our methods to the dolomite system over the full range of compositions and present a wide range of calculated thermodynamic properties and phase diagrams.