A Generalized Solid-State Nudged Elastic Band Method

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I will present a generalized solid-state nudged elastic band (G-SSNEB) method for determining reaction pathways of solid-solid transformations involving both atomic and unit-cell degrees of freedom. This work combines Henkelman el al.'s atomistic NEB [1] with Caspersen and Carter's periodic cell based NEB [2] in an effort to avoid dragging coordinates which can result in a bad reaction coordinate and inaccurate saddle point energies. Atomic and cell degrees of freedom are combined into a unified description of the crystal structure so that calculated reaction paths are insensitive to the choice of periodic cell. For the *rock-salt*–to–*Wurtzite* transition in CdSe, I demonstrate the method is robust for mechanisms dominated either by atomic motion or by unit-cell deformation; notably, the lowest-energy transition mechanism found by the G-SSNEB changes with cell size from a concerted transformation of the cell coordinates in small cells to a nucleation event in large cells. The method is efficient and can be applied to systems in which the force and stress tensor are calculated using density functional theory.

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