Nudged Elastic Band calculations of the hydrogarnet defect in forsterite

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First-principles calculations were performed examining energetic barriers separating different topological configurations of the hydrogarnet defect in Mg_2SiO_4 forsterite using the Climbing Image Nudged Elastic Band (CI-NEB) method. As can be expected hydrogen bonding to oxygen atoms both within the defect and externally plays a fundamental role in the stability of each configuration. Saddle points along the minimum energy path (MEP) typically correspond to the transition of one hydrogen bond breaking to form a new hydrogen bond. MEPs show that out-of-plane torsional hopping of OH bonds can drastically reduce the height of the barrier. We illustrate several different reaction coordinates between symmetry equivalent pairs of configurations and non-symmetry related pairs that also result in an effective means of local charge transport by shifting the center of mass of the 4H cluster. Particularly at low temperatures in the absence of thermally activated processes that result in the breaking of stronger chemical bonds, these types of configurational hopping mechanisms are likely to be important contributors to the bulk electrical conductivity of H_2O-bearing silicate minerals. The barrier heights determined in this study are in good agreement with recent FTIR results of hydrous olivine/forsterite below 600°C. The NEB method can also be used to examine more effective charge and mass transport processes that involve significantly greater atomic displacements.