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Ab initio calculations on point defects in forsterite (Mg_2SiO_4) and implications for diffusion and creep

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ABSTRACT

Ab initio calculations on simple ionic vacancies in forsterite show that there are large energetic differences between vacancies on nonequivalent sites. Oxygen defects on the O3 site are between 1 and 3 eV lower in energy than on the O2 and O1 site, respectively. Magnesium defects on M1 sites are 0.8 eV lower in energy than on the M2 sites. These large energy differences mean that there are many orders of magnitude fewer vacancies on the less-favored sites. In the case of magnesium, where diffusion is thought to occur by means of a vacancy-hopping mechanism, the observed anisotropy with respect to crystallographic orientation can be rationalized by the fact that jumps must only be from M1 to M1 sites