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Vacancy defects in MgO at high pressure

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ABSTRACT

First-principles calculations within the local density and pseudopotential approximations were performed to investigate the effects of pressure on the energetics and structural behavior of charged vacancy defects in MgO. The simulations were performed for a supercell containing 216 atoms with their positions being fully optimized. In particular, the formation and migration energies of cation and anion vacancies were shown to substantially increase over the pressure regime of the Earth's mantle. Our results thus suggest that pressure should suppress intrinsic diffusion mediated by ionic vacancies in MgO over the mantle pressure regime. The calculated three-dimensional data sets for atomic displacements and electron charge density were explored in detail using an interactive visualization system. Although the atomic and electronic structures are highly distorted in the close vicinity of the defects (i.e., in the region covering up to the nearest and next-nearest atoms), the effects are not negligible at farther distances.

Keywords: Defects, mantle minerals, high pressure, rheology, first-principles calculations, scientific visualization