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Energetics of Al doping and intrinsic defects in monoclinic and cubic zirconia : First-principles calculations

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First-principles theory within the supercell approach has been employed to investigate Al doping and intrinsic defects in monoclinic and cubic zirconia. The effect of oxygen chemical potential and Fermi level on the formation energy and on the defect concentration have been taken into account. The formation of oxygen vacancies is found to be energetically more favorable in the cubic than in the monoclinic phase under the same oxygen chemical potential and Fermi energy. In both phases, substitutional Al decays from neutral charge state into the charge state −1, with the transition energy just above to the top of the valence band. Our findings indicate that by confining the Fermi energy to the region between the middle of the band gap and the bottom of the conduction band, high Al solubility could be achieved, although formation of Al is likely followed by the formation of interstitial oxygen. Furthermore, the concentration of Al with charge state −1 along with the equilibrium Fermi energy have been calculated in a self-consistent procedure. Here, the possible compensating defects with the relevant charge states have been considered. The obtained concentrations of Al and oxygen vacancies follow the experimental trend but underestimates experimental data. When the formation of defect clusters, composed by two substitutional Al and one oxygen vacancy, are considered, good quantitative agreement with experimental values of both Al and oxygen vacancy concentration is achieved. The results suggest that defect clusters will be formed as a result of Al doping in cubic phase of ZrO2, whereas the concentration of defect clusters is negligible in the monoclinic phase, both in accordance with experiment.

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