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Ab-initio study of structural stability and electronic structure of monoclinic and cubic ZrO_{2-x}S_xx for 0 ≤ X < 2

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<p>The system ZrO_{2-x}S_xx is limited by the cases ZrO₂ and ZrS₂ (x = 0, 2). Physical properties of such systems for 0 < x < 2 are of great interest, but difficult to obtain from first principles calculation. A recently suggested approach, i.e virtual crystal approximation, allows simulation for changes in composition, while retaining a small unit cell. In this paper we employ Density Functional Theory (DFT) within the Generalized Gradient Approximation (GGA)to study the zirconium dioxide – sulfide system ZrO_{2-x}S_xx, using the CASTEP code. We investigated geometric cell size effects, mechanical properties and electronic structure for these systems at various amounts of sulfur concentrations. For the treatment of solid solutions in the recently introduced VCA approach, CASTEP allows to define partial occupancies for atomic sites; in our case, the anionic lattice sites of ZrO_{2-x}S_xx crystal are defined to be less than fully oxygen occupied: (2-x); and consequently similar sites can then be attributed a partial sulfur character: (x). The lattice parameters and cell size increases for zirconia as the sulfur content is increased. Furthermore, the trend of Fermi level and the electron distributions differ, giving rise to reduced band gap as S is increased. The cubic structure ZrO_{2-x}S_xx is stable for x<1.2, however, the structure gives negative tetragonal shear modulus at x≥1.2, condition of mechanical instability.

Level (Hons, MSc,
   PhD, other)?

MSC

Consider for a student
   award (Yes / No)?

yes

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

no

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