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Ab-initio study of structural stability of monoclinic, tetragonal and cubic ZrO_{2-x}S_x for 0 ≤ X < 2

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Abstract content
   (Max 300 words)

The system ZrO_{2-x}S_x is limited by the cases ZrO₂ and ZrS₂ (x = 0, 2). Physical properties of such systems for 0 < x < 2 are of great interest for catalytic applications, 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. by using first-principle calculations, we employ Density Functional Theory (DFT) within the Generalized Gradient Approximation (GGA) to study the zirconium dioxide – sulfide system ZrO_{2-x}S_x, using the CASTEP code. We investigated geometric cell size effects, mechanical properties and electronic structure for these systems at various 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_x 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 calculated equilibrium lattice parameters and cell size increase for zirconia as the sulfur content is increased,while the calculated single-crystal stiffness, gradually decreases from ZrO₂ to ZrS₂. The cubic structure ZrO_{2-x}S_x is stable for x<1.2, however, the structure gives negative tetragonal shear modulus at x≥1.2; a condition of mechanical instability.Furthermore, the trend of Fermi level and the electron distributions differ, giving rise to reduced band gap as S is increased, At low concentration of sulphur impurity, Zr-O and O-S bond lengths or Zr-S bond lengths are far from equilibrium values, it is obvious that this structures can be considered as stable. at high concentration, the Zr-O and Zr-S bond length are close to equilibrium.

Apply to be
 consider for a student
   award (Yes / No)?

yes

Level for award
 (Hons, MSc,
   PhD)?

MSc

Main supervisor (name and email)
and his / her institution

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Would you like to
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 Proceedings (Yes / No)?

no

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