

Oxygen vacancy, oxygen vacancy–vacancy pairs, and Frenkel defects in cubic lutetium oxide.

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Streszczenie

Electronic and structural properties of cubic Lu_2O_3 with either single oxygen vacancy, oxygen vacancy–vacancy pair, or a Frenkel pair (an oxygen vacancy and an interstitial oxygen) were analyzed using *ab initio* density functional theory calculations. A plane-wave ultrasoft pseudopotential approach with local density approximation functional was used to optimize the geometries. A full-potential linearized augmented plane-wave method with meta-generalized gradient approximation was applied to the optimized geometries to calculate the electronic properties of the systems. Defect-related bands were observed between the valence band and the conduction band. Different charge states of the defects were considered. Both oxygen vacancy and oxygen vacancy–vacancy pairs behave as moderately deep electron traps (trap depth 1.3–2.7 eV). Trapped electron localization at the vacancy site(s) was confirmed using electron density and electron localization function plots. The bands originating from oxygen vacancy–vacancy pairs in Lu_2O_3 exhibit some dependence on the distance between the two entities. The resulting energy differences (considered from an optical absorption point of view) cover ultraviolet, visible, and infrared ranges. Thus, it is plausible that oxygen vacancy–vacancy pairs are responsible for the coloration that is sometimes observed in Lu_2O_3 powders and crystals. On the contrary, the Frenkel pair exhibits no systematic dependence of the defect-related bands on the distance between its oxygen vacancy and interstitial oxygen, while the resulting defect-related bands look similar to those corresponding to the isolated defects. Frenkel pairs are thus considered a probable mechanism of oxygen vacancy formation and stabilization of Lu_2O_3 . Additionally, a brief review of the relevant experimental data is provided in the introduction.

Słowa kluczowe

Oxygen, Defects in solids, Defects, Chemical calculations, Mathematical methods

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