

Defects in hafnium-doped lutetium oxide and the corresponding electron traps: a meta-generalized gradient approximation study

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A number of Lu_2O_3 -based materials were reported to present efficient capability of trapping excited charge carriers in metastable excited states formed either by specific dopants or naturally occurring defects. Over the years, abundant experimental data have been collected, which were taken as a solid ground to treat the problem using computational chemistry. Density functional theory (DFT) calculations with an advanced meta generalized gradient approximation (mGGA) functional were used to analyze electron trapping in cubic Lu_2O_3 doped with Hf. Individual ions of dopant and nearest-neighbor dopant ion pairs were considered. The effects of interstitial anions such as O^{2-} and Cl^- were analyzed. In most of the analyzed cases the additional electron charge is localized at the dopant site. However, in many of the studied cases, the dopant/defect states overlap with the conduction band and cannot correspond to electron trapping. The Hf^{3+} ion in the Lu site of C_{3i} local symmetry (O_h) corresponds to a moderate trap depth of 0.8–0.9 eV. Several composite defects corresponding to deeper (1.1–1.4 eV) traps also exist. Unambiguous deep traps (1.5–1.8 eV) correspond to systems with Hf dopant in the cationic void, accompanied by two interstitial oxygen atoms. The results thus indicate that basic 'Hf-substitutes-Lu' doping is unlikely to correspond to the deep traps observed experimentally in $\text{Lu}_2\text{O}_3:\text{Tb},\text{Hf}$ and $\text{Lu}_2\text{O}_3:\text{Pr},\text{Hf}$ and more complex defects must be involved.

Słowa kluczowe

thermoluminescence, trap depth, meta-gga, hafnium, lutetium oxide

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