Defect states in cubic lutetium oxide caused by oxygen or lutetium inclusions or vacancies.

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Streszczenie

Effects of defect introduction on electronic structure of cubic Ia-3 lutetium oxide (Lu2O3) were characterized bymeans of density-functional theory calculations using augmented plane wave method with local orbitals (APW+LO) approach. Perdew-Wang 92 local density approximation (LDA) and Räsänen, Pittalis, and Proetto meta-generalized gradient approximation (meta-GGA) density functionals were used. It was found that interstitialoxygen (introduced into the oxygen void available in the structure) and lutetium vacancies result in defect stateslocated about 0.1–0.8 eV above valence band, which can act as hole traps. Oxygen vacancy can act as efficientelectron trap, with depth about 1.25 eV. Interstitial lutetium in either C3ication void or in oxygen void results instates located about 0.2–1 eV below conduction band, which can act as electron traps. Both interstitial Lu and Luvacancies create multiple traps of different depths, which might contribute to experimentally observed trapdistributions in Lu2O3

Słowa kluczowe

Lutetium oxide, APW+LO, Defects, Carrier trapping, Thermoluminescence

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