

Meta-generalized gradient approximation time-dependent density functional theory study of electron trapping in Hf- and Zr-doped lutetium oxide: influencing the oxygen vacancy

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Streszczenie

This work analyzes the effects of a nearby Hf or Zr dopant on the electron density trapped at an oxygen vacancy site. The two metals are among the dopants used to achieve thermoluminescence and energy storage in phosphors based on cubic lutetium oxide (c-Lu₂O₃). The presence of oxygen vacancies is anticipated in those phosphors. If the dopant is located outside the immediate surroundings of the vacancy site, the resulting optical trap depth is similar to that of the isolated oxygen vacancies (1.6-1.7 eV versus 1.7 eV). If the dopant is one of the four metal cations surrounding the vacancy site, the corresponding trap depth is 2.0-2.1 eV. Using time-dependent density-functional theory calculations, it was found that the excitation of the vacancy-trapped electrons can take two forms: a local excited state at the vacancy site can be formed, or an electron transfer to Hf might occur. With charge compensation in mind, several structures with three defects were analyzed: the dopant cation, the vacancy and an interstitial oxygen (Hf/Zr plus a Frenkel pair). These last two systems with the dopant in a +4 oxidation state and a single electron trapped at the vacancy site correspond to zero total charge, while another electron can be trapped. The vacancy site is expected to trap the electron, not the dopant. The composite defects of the dopant and Frenkel pair are thus considered the most likely electron traps in cubic Lu₂O₃:Hf and cubic Lu₂O₃:Zr.

Słowa kluczowe

TD-DFT, meta-GGA, meta-generalized gradient approximation, storage phosphors, thermoluminescence, time-dependent density-functional theory, trap depth

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