

Abstract Submitted
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First-principle study of phosphors for white-LED applications : absorption and emission energies for Ce- and Eu-doped hosts.¹ XAVIER GONZE, YONGCHAO JIA, ANNA MIGLIO, MATTEO GIANTOMASSI, Universit catholique de Louvain, Belgium, SAMUEL PONCE, Oxford University, UK, MASAYOSHI MIKAMI, MCHC RD Synergy Centre, Inc, Yokohama, Japan — After the invasion of compact fluorescent lamps, white LED lighting is becoming a major contender in ecofriendly light sources, with a combination of yellow-, green- and/or red-emitting phosphors partly absorbing the blue light emitted by an InGaN LED. After introducing the semi-empirical Dorenbos model for 4f 5d transition energies of rare earth ions, I present a first-principle study of two dozen compounds, pristine as well as doped with Ce³⁺ or Eu²⁺ ions, in view of explaining their different emission color. The neutral excitation of the ions is simulated through a constrained density functional theory method coupled with a delta SCF analysis of total energies, yielding absorption energies. Then, atomic positions in the excited state are relaxed, yielding emission energies and Stokes shifts, and identification of luminescent centers. In case of the Ce doped materials, the first-principle approach matches experimental data within 0.3 eV for both absorption and emission energies, covering a range of values between 2.0 eV and 5.0 eV, and provides Stokes shifts within 30%, with two exceptions. This is significantly better than the semi-empirical Dorenbos model. A similar analysis is performed for Eu-doped materials, also examining the thermal quenching of two oxynitride hosts.

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