Combined theoretical-experimental study of chromium doped zinc gallate phosphor

Arthur De Vos[a,b], Danny E.P. Vanpoucke[a], Kurt Lejaeghere[a], Jonas J. Joos[b], Philippe F. Smet[b], Karen Hemelsoet[a]

[a] Center for Molecular Modeling, Ghent University, Technologiepark 903, 9052 Zwijnaarde Belgium
[b] LumiLab, Ghent University, Krijgslaan 281, S1, 9000 Ghent, Belgium

arthur.devos@ugent.be

Persistent phosphors form an interesting group of materials with a variety of applications. To date, many questions remain on the precise physical processes responsible for their particular luminescent behavior. A combination of theory and experiment is suited to gain a deeper understanding.

This theoretical study investigates the persistent phosphor, zinc gallate doped with chromium (ZGO:Cr), through periodic density-functional theory simulations [1, 2]. The dopant, Cr^{3+}, inside the inorganic host crystal and its interactions determine the luminescent behavior of this persistent phosphor. The stability of the dopant on different sites is investigated and the electronic structure is calculated. The introduction of an antisite defect, a configuration where two cationic elements of the host material are exchanged, creates an electrical field that is important for the proposed trapping mechanism [3, 4]. The effect of an antisite defect on the spectroscopic and electronic properties is examined together with its stability. The density of states is calculated for these different materials and is used to explain the interactions between states and the experimentally measured excitation bands.

Keywords—Spectroscopy, $ZnGa_2O_4:Cr^{3+}$, density-functional theory, experiments

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