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Ab initio Simulation of Y2O3 -Doped Cerium Using Heyd–Scuseria–Ernzerhof HSE Hybrid Functional and DFT+U Approaches

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Abstract : It is known that Y2O3 Material is the most important among the sesquioxides within the general class of refractory ceramics. Indeed, this compound has many applications such as sintering optical windows, components for rare-earth doped lasers as well as inorganic scintillators in the detection scintillation. In particular Eu2+ and Ce3+ are favored dopants in many the scintillators due to its allowed optical 5d-4f transition. In this work, we present new results concerning structural and electronic properties of Ce-doped Y2O3, investigated by density functional theory (DFT), using the Heyd–Scuseria–Ernzerhof (HSE) hybrid functional and DFT+U two approaches. When, we compared the results from the two methods we obtain a good agreement available experimental data. Furthermore, the effect of cerium on the material has also been studied and discussed in the same framework.

Keywords : DFT, vienne ab initio simulation packages, scintillators, Heyd–Scuseria–Ernzerhof (HSE) hybrid functional
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