

## **Accounting oxygen vacancy for half-metallicity and magnetism in Fe-doped CeO<sub>2</sub> dilute magnetic oxide**

### **Abstract**

The present work explores the electronic and magnetic properties of Ce<sub>1-x</sub>Fe<sub>x</sub>O<sub>2</sub> ( $x = 0.125$  and  $0.06$ ) with and without oxygen vacancies by full potential linear augmented plane wave method (FPLAPW) based on density functional theory (DFT). An on-site Coulomb correction to the standard generalized gradient approximation (GGA) is used to describe exact exchange-correlation potential. The resulting GGA+U formalism, leads to the results comparable to realistic experiment. The calculated results show that the doping of Fe-atom induces the ferromagnetism in CeO<sub>2</sub> with and without oxygen vacancy. Moreover, the studied compound retains half metallicity at both dopant concentrations with 100% spin polarization at Fermi level ( $E_F$ ). The emergence of ferromagnetism in it with/without oxygen vacancy can be attributed to F-center mechanism/double exchange mechanism.

**Keywords** — DFT, DMS, FPLAPW method, GGA+U, spintronics