



# GEMaC

## Groupe d'Étude de la Matière Condensée

# ISSUES WITH DENSITY FUNCTIONAL THEORY FOR DESCRIBING DEFECTS AND DOPANTS IN METAL OXIDES

**This seminar is a presentation by Dr. Michael NOLAN showing the work on cerium dioxide and titanium dioxide, with DFT corrected for on-site Coulomb interactions, DFT+U, to study oxygen vacancy formation, metal adsorption and the defects that form upon doping.**

le mardi 25 mai 2010 à 14h30

Département de Physique

Bâtiment Buffon Salle 212

GEMAC, antenne de Versailles, 45, Av.  
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Defects and dopants in metal oxides are absolutely crucial to their performance in many applications. Modelling of defect formation and doping is an important part of

understanding these processes. The most widely used approach is density functional theory (DFT). However, due to limitations in present approximate exchange-correlation functionals, e.g. the local density and generalised gradient approximations, the DFT description of many defects and dopants in widely used metal oxides is, in the main, entirely incorrect.

We present some results from our work on cerium dioxide and titanium dioxide, where we have used DFT corrected for on-site Coulomb interactions, DFT+U, to study oxygen vacancy formation, metal adsorption and the defects that form upon doping. In general, the DFT+U results are consistent with known experimental data and can also be used to predict the cation oxidation states present upon doping, as well as rationalising experimental findings.

However, DFT+U has its own limitations, principally, that the U parameter is empirical and that U can only be applied to particular species. To this end, we have begun hybrid DFT studies of defects and dopants in metal oxides and present some initial results on this to assess the applicability of DFT+U.

## INFORMATIONS COMPLÉMENTAIRES

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