Contribution submission to the conference Dresden 2014

Is Cerium Unique? Rare Earth Metals in Density-Functional Theory — •Marco Casadei[1], Xinguo Ren[2], Patrick Rinke[1], Angel Rubio[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Technology, Hefei, China — [3]University of the Basque Country, Donostia, Spain

The presence of f electrons in the rare earths and their interaction with the s and p electrons give rise to a plethora of physical phenomena. One prominent example is the isostructural α-γ phase transition in cerium (Ce). We have shown that density-functional theory (DFT) captures the volume collapse associated with the transition, but only if advanced density functionals such as exact exchange plus correlation in the random-phase approximation (EX+cRPA) are used [1]. The volume collapse is understood in terms of a *localization/delocalization* of the f electrons. The question we then addressed by applying DFT also to lanthanum (La), praseodymium (Pr) and neodymium (Nd) is, *is the isostructural volume collapse in cerium unique*? All these elements undergo several structural changes with pressure. We find that the structural transitions are already captured at a lower level of DFT (i.e. with (semi)-local functionals) and therefore conclude that f-electrons are not the driving force in this case. Within hybrid functionals, we find only one phase in lanthanum, which has no f-electrons, and more than one stable solution in the fcc crystal structure for Pr and Nd, as found for Ce. Unlike in Ce, however, the curves are nested and thus no isostructural volume collapse emerges in agreement with experiments.
[1] M. Casadei *et al.*, Phys. Rev. Lett. **109**, 14642 (2012).

Part:	**O**
Type:	**Vortrag;Talk**
Topic:	**Focussed Session: Frontiers of Electronic Structure Theory**
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