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Density-Functional Theory Applied to Rare Earth Metals: Approaches Based on the Random-Phase Approximation MARCO CASADEI, XINGUO REN, PATRICK RINKE, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany, ANGEL RUBIO, Nano-Bio Spectroscopy group and ETSF, Universidad del Pais Vasco, UPV/EHU, Avenida de Tolosa 72, E-20018, Donostia-San Sebastian, Spain — The description of the volume collapse present in some of the *rare earth* metals poses a great challenge to density-functional theory (DFT) since local/semilocal functionals (LDA/GGA) fail to produce the associated phase transitions. We approach this problem by treating all electrons at the same quantum mechanical level. The calculations are performed on cerium and praseodymium, that display a volume collapse, and neodymium, in which the volume collapse is absent, using both hybrid functionals (e.g. PBE0 and HSE06) and exact-exchange plus correlation at the level of the random phase approximation (EX+cRPA). The performance of recently developed beyond RPA schemes (e.g. rPT2 [1]) is also tested on these f electron systems. For the isostructural α - γ phase transition in cerium PBE0 and HSE06 produce two distinct solutions that can be associated with the α and γ phases. The structural and magnetic properties are in agreement with experiment, but the relative energetic order is wrong. EX+cRPA is essential to correct this failure and achieves quantitative agreement with the extrapolated phase diagram [2]. [1] Ren *et al.* (to be published). [2] M. Casadei *et al.*, Phys. Rev. Lett. **109**, 14642 (2012).

Prefer Oral Session

Prefer Poster Session

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