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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 MPG, Berlin, Germany, ANGEL RUBIO, University of the Basque Country UPV/EHU, Donostia, Spain — The description of the volume collapse exhibited by some *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, using both hybrid functionals (e.g. PBE0 and HSE06) and exact-exchange plus correlation in the random-phase approximation (EX+cRPA). We also assess the performance of recently developed beyond RPA schemes (e.g. rPT2 [1]). The calculations are performed for cerium and praseodymium, that display a volume collapse, and neodymium, in which the volume collapse is absent. The isostructural α-γ phase transition in cerium is the most studied. The exact exchange contribution in PBE0 and HSE06 is crucial to produce two distinct solutions that can be associated with the α and γ phases, but quantitative agreement with the extrapolated phase diagram requires EX+cRPA [2].

[1] Ren *et al.*, J. Mater. Sci. **47**, 7447 (2012).
[2] M. Casadei *et al.*, Phys. Rev. Lett. **109**, 14642 (2012).

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