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Magnetic properties and exchange interactions in transition metal oxides: Benchmarking the ACBN0 functional PRIYA GOPAL, Central Michigan University, MI, MARTA GUSMAO, Federal University of Amazonas, Manaus, Amazonas, Brazil, RABIH ORABI, Central Michigan University, MI, STEFANO CURTAROLO, Duke University, MARCO FORNARI, Central Michigan University, MI — We study the magnetic properties and magnetic exchange interactions in the 3d transition metal (TM= Mn, Co, Fe and Ni) oxides using the recently developed ACBN0 functional which is a parameter-free extension of traditional DFT+U functional where the Hubbard U is calculated selfconsistently and depends on the electron density of the system.ACBN0 greatly improves the electronic properties of the TMOs by improving the band-gap in MnO and NiO and making CoO and FeO insulating which is otherwise described incorrectly within DFT (LDA/GGA) functionals. The magnetic properties (magnetic moments, magnetic ordering energies, exchange coupling constants (Js)) are all better described by ACBN0 at par with the Hybrid functionals and in closer agreement with the experimental values. For MnO and NiO, we investigated the magnetic properties at equilibrium and under pressure and found a good agreement with other advanced functionals. For all the oxides studied here, we did a thorough and e xtensive study by comparing different pseudopotentials and find overall that ACBN0-LDA is better for describing magnetic properties compared to ACBN0-PBE. We also discuss the application of ACBN0 to two mixed-valent systems Mn_3O_4 and Co_3O_4, where it is possible to evaluate U for different sites.

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