

Abstract Submitted
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Examining the density functional theory description of VO₂ above and below the metal-insulator transition¹ RICARDO GRAU-CRESPO, THOMAS A. MELLAN, Department of Chemistry, University College London, UK, HAO WANG, UDO SCHWINGENSCHLÖGL, KAUST, PSE Division, Saudi Arabia — Vanadium oxide (VO₂) exhibits a metal-insulator transition at 341 K, which is accompanied by a change from a tetragonal to a monoclinic structure. We examine the electronic and magnetic properties of VO₂ below and above the transition point, as calculated from density functional theory (DFT) and some extensions, including hybrid DFT / Hartree-Fock functionals and Hubbard-corrected functionals. We show that the groundstate solutions obtained with either the GGA approximation or the screened hybrid functional HSE (25% of Hartree-Fock exchange) are at odds with experimental observations for both phases. We then discuss the effect of varying amounts of Hartree-Fock exchange and values of the Hubbard parameter U on the solutions. Although the agreement of some of the calculated properties with experiment can be tuned in this way, we conclude that no single setting can describe the properties of both VO₂ phases simultaneously.

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