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Bulk and surface properties of rutile TiO_2: an ACBN0 case study LAALITHA LIYANAGE, University of North Texas, PRIYA GOPAL, Central Michigan University, LUIS AGAPITO, University of North Texas, MARCO FORNARI, Central Michigan University, STEFANO CURTAROLO, Duke University, MARCO BUONGIORNO NARDELLI, University of North Texas — Using the newly developed Agapito–Curtarolo–Buongiorno–Nardelli (ACBN0) functional[1] we investigate bulk and surface properties of rutile TiO_2. ACBN0 is a pseudo-hybrid Hubbard density functional that is a fast, accurate and parameter-free extension of traditional DFT+U that has been proved to correct both the band gap and the relative position of the different bands in transition metal compounds. Within ACBN0, the values of U and J are functionals of the electron density and depend directly on the chemical environment and crystalline field, thus providing a direct way of computing the Hubbard corrections for any individual atom in any local environment. With rutile TiO_2 as a stringent test-bed, we have applied ACBN0 to the evaluation of a broad range of physical and electronic properties of the bulk and surfaces ((100), (110), and (001)), including electronic structure, vacancy formation energy, surface formation energy and water adsorption energy. Our results compare favorably with existing GGA, traditional GGA+U and hybrid functional calculations, demonstrating the versatility and accuracy of the ACBN0 approach.

[1]L. Agapito, S. Curtarolo, M. Buongiorno Nardelli, arXiv:1406.3259

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