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Elucidating the Band Gap of Niobium Dioxide ANDREW O'HARA, The University of Texas at Austin, DEREK VIGIL-FOWLER, STEVEN G. LOUIE, University of California - Berkeley and Lawrence Berkeley National Lab, ALEXANDER A. DEMKOV, The University of Texas at Austin — Like VO_2, niobium dioxide (NbO_2) belongs to the family of transition metal oxides with a temperature-driven metal-to-insulator transition. However, NbO_2 has received considerably less attention, and several open questions about the material remain. One such question, of both practical and fundamental importance, is the nature and size of the band gap in the low-temperature, distorted rutile phase with a range reported for the gap of 0.5 eV to 1.2 eV. In this work, we investigate the low-temperature phase, utilizing several methodologies - density functional theory within the standard local density approximation (LDA), LDA+U, hybrid functional, and the GW approximation, to better understand the physics of the band gap in NbO_2. Comparisons of the calculations are made to recent experimental work on NbO_2 utilizing photoemission spectroscopy and ellipsometry. This work is supported by DOE under the SciDAC program, the NSF, and SRC.

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