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Investigation of the Band Gap in Co_3O_4 MARK SHOLTE, CHUNG-WEI LIN, KRISTY KORMONDY, University of Texas System, TIMOTHY NUNLEY, New Mexico State University, AGHAM POSADAS, University of Texas System, STEFAN ZOLLNER, New Mexico State University, ALEXANDER DEMKOV, University of Texas System — Co_3O_4 is a strongly correlated oxide with a spinel structure and G-type antiferromagnetic order at temperatures below 40 K. It is a widely studied material owing to its applications in gas sensing, spintronics, batteries, and catalysis. The strong correlation and magnetism make it a difficult material to model from first principles. Density functional theory calculations require the use of a Hubbard U to correctly model its magnetic behavior. The band gap is sensitive to the choice of U allowing one to tailor the gap to a wide range of values. This often provides a phenomenological approach to determining U, but in the case of Co_3O_4 there is no experimental consensus on the actual value of the band gap. We utilize an alternate approach by matching the theoretical valence band structure to the actual valence band data obtained via x-ray photoemission spectroscopy. This generated set of U values is used to compute an absorption spectrum, which is in good agreement with ellipsometry results.

Mark Sholte
University of Texas System

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