Abstract Submitted
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Quasiparticle Energies in Pristine and Oxygen Depleted MoO3 for Pseudocapacitor Applications[1] KEITH RAY, University of California, Berkeley, HAO LIN, VIDVUDS OZOLINS, University of California, Los Angeles, MARK ASTA, University of California, Berkeley — Alpha-MoO3 is a promising electrode material for pseudocapacitors, devices that store electrical energy faradaically, but feature fast reactions/intercalations enabling high power applications [1]. Electrical conductivity and optical properties in alpha-MoO3 are strongly affected by defects, such as oxygen vacancies, which affect the electronic structure. Utilizing self-consistent GW calculations in the quasiparticle picture, along with G0W0 calculations with starting orbitals from HSE06 and DFT+U, we calculate the electronic structure of pristine and oxygen depleted alpha-MoO3. We focus on the sensitivity of our results to the calculated description of the localized d-electron states and compare with band gap values determined by measurements on optical properties, electrical conductivity, and photoemission spectroscopy from the literature.

[1] T. Brezesinski, J. Wang, S. H. Tolbert and B. Dunn, Nature Materials 9, 146 (2010)

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