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Effect of doping and chemical ordering on the optoelectronic properties of complex oxide semiconductors IFFAT NAYYAR, CHAMBERLIN SARA, TIFFANY KASPAR, Physical Sciences Division, Pacific Northwestern National Laboratory, NIRANJAN GOVIND, Environmental and Molecular Sciences Laboratory, Pacific Northwestern National Laboratory, SCOTT CHAMBERS, Physical Sciences Division, Pacific Northwestern National Laboratory, PETER SUSHKO, Physical Sciences Division, Fundamental and Computational Sciences Directorate, Pacific Northwestern National Laboratory — Transition metal oxide hematite, α-Fe_2O_3, is of interest in photovoltaic and photoelectrochemical applications due to its natural abundance, narrow band gap and electrochemical stability. Doping of α-Fe_2O_3 may lead to conductivity enhancement and band-gap reduction. In this work, we have studied the electronic and optical properties of α-$(Fe_{1-x}V_x)_2O_3 (0 \leq x \leq \sim 0.5)$ solid-solution epitaxial thin films using advanced theoretical models employing embedded cluster approach and time-dependent density functional theory. We observe that V doping results in localized, occupied V *3d* states which are hybridized with Fe *3d* and are located in the midgap of pure α-Fe_2O_3. The lowest energy transitions for α-$(Fe_{1-x}V_x)_2O_3$ films are the electronic excitations from these levels to the unoccupied Fe $3d^*$ orbitals, reducing the onset of α-Fe_2O_3photoconductivity by nearly 1.2 eV. Our calculated optical absorption spectra are in good agreement with the experiment. This insight into the atomic, electronic and spin ordering provides guiding principles for the design of new oxide semiconducting materials for efficient visible light harvesting, thus enabling the technological growth of alternate energy sources for solving the renewable solar energy and photo-chemical organic waste remediation problems.

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