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Electronic, magnetic, and optical properties of Semiconducting Spinel Fe_2CrO_4[1] TIM DROUBAY, TIFFANY KASPAR, IFFAT NAYYAR, Pacific Northwest National Laboratory, DAVID KEAVNEY, Advanced Photon Source, PETER SUSHKO, SCOTT CHAMBERS, Pacific Northwest National Laboratory — Transition metal oxides offer significant flexibility in tailoring functional properties by virtue of the high degree of solid solubility of different cations within the host lattice. For instance, the electronic properties of magnetite (Fe_3O_4), a ferrimagnetic half metal, can be substantially changed by substituting one third of the Fe cations with Mn, Ni, Co, Zn or Mg. The actual magnetic properties of any given ferrite depend critically on whether the dopant occupies the tetrahedral (A) or octahedral (B) sites, or a mix of the two. Doping magnetite to produce a ferromagnetic semiconductor would be of considerable interest for spintronics and photocatalysis, particularly if the bandgap remains small. The detailed functional properties depend on the local structure, which is dictated in large measure by the cation sublattice(s) the dopants occupy, the valence(s) they exhibit, and the relative energy scales of competing effects, including short-range disorder, that determine the overall electronic structure. We have investigated Cr as the dopant in Fe_3O_4 by carrying out epitaxial film growth by molecular beam epitaxy and characterization, along with first principles modeling to explore new model materials. We find that replacing 1/3 of the Fe atoms with Cr atoms results in a low-gap, thermally robust ferrimagnetic semiconductor that is photoconductive in the visible, whereas replacing 2/3 of the Fe with Cr produces an insulator with no net magnetization.

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