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Oxygen vacancies and ferromagnetism in Co-doped anatase¹

JOHN JAFFE, TIMOTHY DROUBAY, SCOTT CHAMBERS, Pacific Northwest National Laboratory — Cobalt-doped titanium dioxide, or CTO, has emerged in the past few years as a semiconducting, transparent, room-temperature ferromagnet. Very recently it has been shown that the magnetism in anatase-structure CTO often originates in surface nanoparticles or Co-rich regions that have a much-enhanced substitutional Co content up to 40% of Ti sites, so that magnetic CTO is not a true dilute magnetic semiconductor (DMS), but rather a fairly high-density spin system. In this work we describe a computational study of Co-rich CTO using the Generalized Gradient Approximation (GGA) to density functional theory (DFT) within the supercell model. Our total energy calculations show a strong tendency for Co-atom clustering or segregation on Ti sites. There is also a strong tendency for the oxygen vacancies to form complexes with the Co atoms. In addition, we find that the oxygen stoichiometry plays an essential role in determining the system's magnetic order. The largest ordered moments require at least enough oxygen vacancies to put all of the Co atoms in the +2 charge state, as they indeed appear to be experimentally, so that the conventional DMS mechanism could only apply via n-type carriers. We find a small but not negligible spin density associated with Ti atoms near the vacancy sites, suggesting an F-center-mediated interaction between the much larger Co moments.

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