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Spin-driven transition metal clustering in the wide-gap ferromagnetic semiconductor Cu_2O:Co[1] HANNES RAEBIGER, STEPHAN LANY, ALEX ZUNGER, National Renewable Energy Lab., Golden CO 80401 — Cu_2O is a prototype material for p-type transparent conductive oxides, and a host material for diluted magnetic semiconductors. Using local density-functional supercell calculations we study (1) the origin of p-type behavior of pure Cu_2O, and (2) the short and long range magnetic interactions of Co atoms substituting Cu. We find that (i) Cu vacancies produce holes, which O vacancies are not able to destroy thus explaining the natural p-typeness, (ii) a single Co induces a fully occupied and localized level near midgap. This would suggest Co–Co magnetic interactions to be weak because there is no energy gain in magnetic coupling. Nevertheless, (iii) we find that Co–Co pairs lead to a huge ferromagnetic stabilization energy and binding energy, both of around 0.5 eV/pair. This dimerization is accompanied by strong lattice relaxation and symmetry breaking together with level splitting. Both clustering and ferromagnetism are caused by the fact that the bonding states of the previously unoccupied levels become occupied and are lower in energy relative to the antibonding levels of previously occupied levels. Such binding is allowed only for Co atoms with the same spins, leading to ferromagnetism (albeit short ranged).

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