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Multifarious-magnetism in copper oxide nanostructures from first-principles X.-Y. CUI, A. SOON, University of Sydney, B. DELLEY, Paul Scherrer Institut, S.-H. WEI, National Renewable Energy Laboratory, C. STAMPFL, University of Sydney — Driven by the ever-increasing demand for novel spin-dependent advanced materials, investigation of nanoscale magnetic materials is currently actively pursued. With the latest developments focusing more on magnetic semiconducting oxides, materials based on cuprous oxide, Cu_2O, are of high interest as potential *p*-type semiconducting candidates. Thus developing an understanding of how intrinsic defects influence both its electronic and magnetic properties is important. We perform density-functional theory calculations [1] and analyze both the electronic and magnetic properties of native defects in both bulk Cu_2O and its surfaces, as well as their respective formation/surface energies under different growth conditions. We find that under oxygen-lean conditions, the experimentally observed ferromagnetic behaviour [2] could originate from copper vacancies on $Cu_2O(111)$ while under oxygen-rich conditions, low energy bulk oxygen interstitials might explain the ferromagnetic moment found in the same material. This suggests that the origin of observed magnetism in sub-stoichiometric copper oxide nanoparticles could be multifarious, highlighting the complimentary role of bulk and surface native magnetic defects.

[1] A. Soon *et al.* submitted
[2] A. Ye. Yermakov*et al.* J. Magn. Magn. Mater. **310**, 2102 (2007)

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