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# Revealing a room temperature ferromagnetism in cadmium oxide nanoparticles: An experimental and first-principles study

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**Experimental details.** The starting material in the present work is cadmium acetate dehydrate [$Cd(CH_3COO)_2.2H_2O$], (sigma-aldrich products). An amount from the complex put in open ceramic crucible was flash sintered in air in a furnace at temperature 500$^{o}$C for 1 hour for dissolving and crystallization and then naturally cooled with the furnace to RT. Some of the yielded powder was further annealed in vacuum of better than $10^{-3}$ torr at ~ 400$^{o}$C for 4 hours and cooled naturally to room temperature (RT) in vacuum. Another amount of the prepared powder was also further heated inside a tightly closed flak filled with hydrogen gas under atmospheric pressure at 350$^{o}$C for 1 hour and cooled with $H_2$ gas for 1h outside the furnace before exposing the powder to air. Finally, the resulting powders were grounded and pelletized using 750 MPa.

Structural analyses were performed using the Rigaku Ultima IV $\theta$-$2\theta$ X-ray diffraction (XRD) equipment with Cu $K_\alpha$ radiation (0.15406 nm) and a step size of 0.04°. Elemental contents and purity were examined with energy dispersion x-ray fluorescence (EDXRF) spectroscopy method by using a sensitive Amptek XR-100CR detector. Magnetic characterization was made using a vibrating sample magnetometer type Micro-Mag Model 3900 with a sensitivity of 0.5 emu for a 1 s averaging time scale. Magnetization curves were measured at room temperature (T=294 K) from +1 to -1 T.

In order to perform a high-resolution TEM (HR-TEM) analysis of samples, FEI TEM instrument Titan G2 80-300 ST was used, which equipped with an energy-dispersive spectroscopy (EDS) detector and a charged couple devices (CCD) camera. TEM analysis was completed by operating the microscope at 300 keV electron beam energy. Figure S1 demonstrates the energy-dispersive X-ray fluorescence (EDXRF) spectrum for the synthesised CdO powder. The spectrum shows only Cd L-spectrum (3.13 - 3.53 keV) with weak exciting signals Cu $K_\alpha$ and $K_\beta$-signals 8.04 keV and 8.90 keV, respectively referring to the excellent purity of the studied samples.

**Computational details.** Our DFT calculations were performed using the SIESTA package [1] with numerical atomic orbital basis sets [2] and Troullier–Martins norm conserving pesudopotentials [3]. We employed the generalized gradient approximation Perdew–Burke–Ernzerhof [4] (GGA-PBE) for the exchange–correlation functional. The optimized double-ζ plus (DZP) polarization basis set with an extra diffuse function was employed for metals. The orbital energy shift parameter that defines the confinement radii of different orbitals, $\Delta E_{PAO}$ was

considered to be 50 meV. This value gives a rather good precision within the accuracy of the GGA+U used functional [5]

The energy cutoff for the real space grid used to represent the density was set as 150 Ry. The Quasi-Newton l-BFGS method was employed for geometry relaxation until the maximal forces on each relaxed atom were less than 0.03 eV $Å^{-1}$ and a criterion of 0.01 eV $Å^{-1}$ has been utilized to achieve a full convergence of the energy of a nanoparticle larger than 2 nm. In order to improve the description of electronic correlations in the Cd-d shell, an on-site Coulomb interaction of U = 4.5 eV was taken into account. The starting structure of CdO nanoparticles (NP) is modeled as a Wulff construction [6] of faceted CdO nanocrystal, although no symmetry was enforced in the calculations as shown in Figure S2. Furthermore, we saturate the dangling surface bonds by H-passivation [7].

**References**

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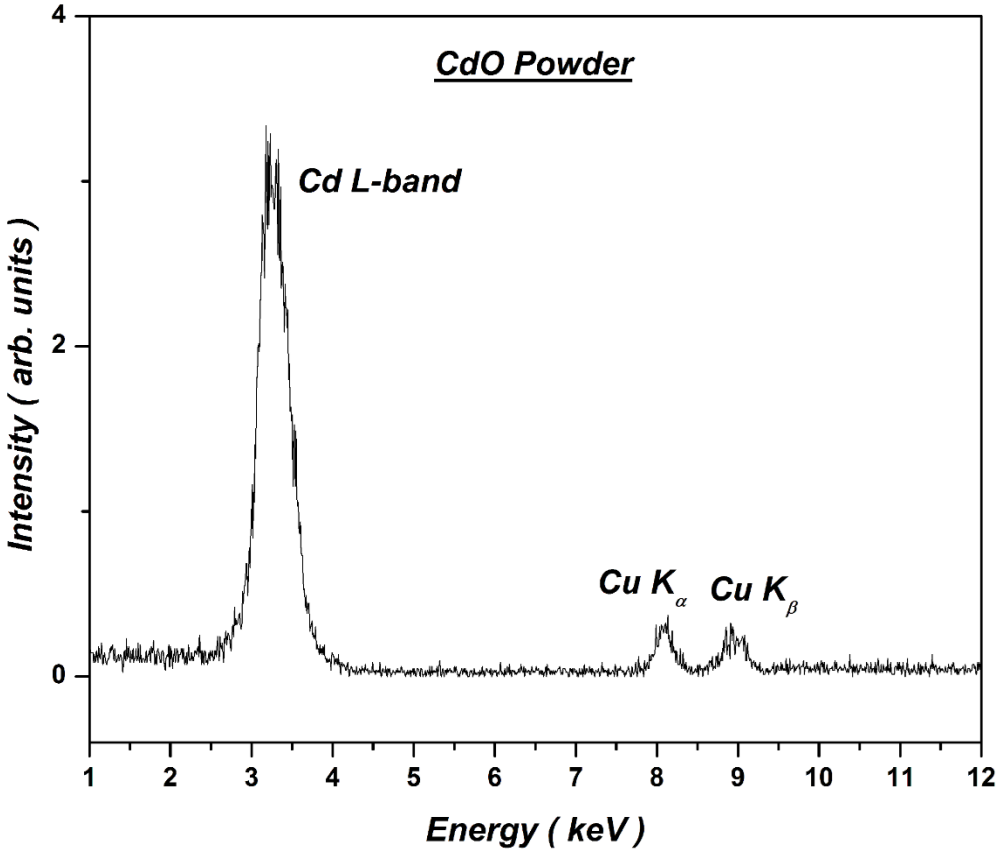


**Figure S1**. X-ray fluorescence of synthesized CdO powder.

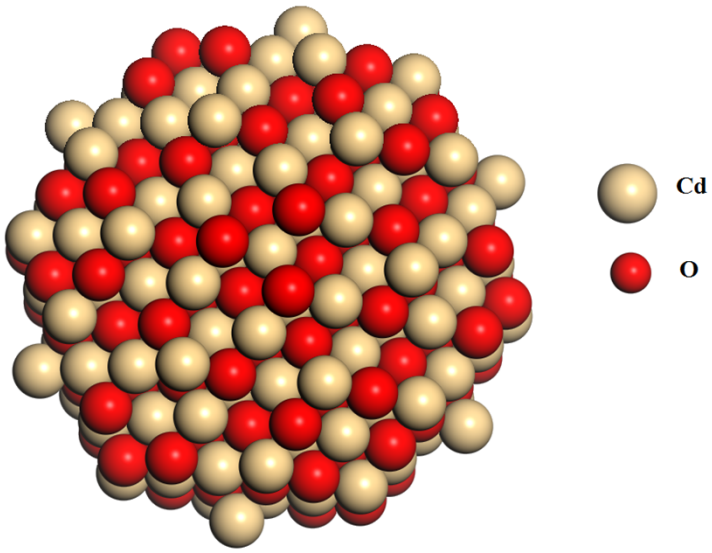


**Figure S2**. CdO nanoparticle, containing 341 atoms constructed by Wulff scheme, and used in DFT calculations.