Effect of oxygen point defects on electronic and magnetic properties of copper pyrophosphate material.

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Based on density functional theory (DFT), we investigate the oxygen point defects (V-vacancy, V_I- interstitials) impact on the electronic and magnetic properties of copper pyrophosphate dihydrate (CuPPD) material. Calculations were performed with the generalized gradient approximation (GGA) of the exchange-correlation functional (E_{xc}) supplemented by strong Coulomb interaction via Hubbard-like Hamiltonian (U). The GGA+U method was applied for Cu-3d and O-2p states. The results show that oxygen atom vacancy defect induced the decrease of a magnetic moment from U=8.66 to 7.02 and 7.84 μB/cell for vacancy and interstitials defect, respectively. The magnetic moment mainly comes from the Cu atom d orbitals. Furthermore, our calculations reveal that oxygen vacancies strongly modified the electronic structure of CuPPD by inducing non-zero density of states (from Cu-3d and O-2p state) near the Fermi level. As a result, a significant reduction in the electronic band gap of our material can be noticed. The findings of this study provide insight into modified by defects electronic properties of semiconductor-like CuPPD crystal. This issue is of interest to nanoelectronics and the production of nanomaterials, including quantum dots [1].

References:

[1] Laskowski, Ł.; Majtyka-Piłat, A.; Cpałka, K.; Zubko, M.; Laskowska, M. Synthesis in Silica Nanoreactor: Copper Pyrophosphate Quantum Dots and Silver Oxide Nanocrystallites Inside Silica Mezochannels. Materials 2020, 13, 2009.