Abstract Submitted
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Photoelectron spectra of copper oxide ($Cu_xO_y^-$, $x = 1-2$, $y = 1-4$) clusters from first principles[1] BIN SHI, University of Illinois at Chicago, SHIRA WEISSMAN, Weizmann Institute of Science, LINDA HUNG, University of Illinois at Chicago, LEEOR KRONIK, Weizmann Institute of Science, SERDAR OGUT, University of Illinois at Chicago — Copper oxide clusters are systems of both technological and fundamental interest. They have unique electronic and optical properties due to the exchange and correlation effects of their d electrons, which also make their modeling from first principles computationally demanding. We optimize the ground-state structures of copper oxide $Cu_xO_y^-$ ($x = 1-2$ and $y = 1-4$) cluster anions using density functional theory (DFT). We compare photoelectron spectra determined at two levels of theory: DFT and the GW approximation. DFT calculations use Perdew-Burke-Ernzerhof (PBE), hybrid, and range-separated exchange-correlation functionals. The calculated photoelectron spectra are compared with available experimental measurements to identify the nature of the observed electronic excitations.

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