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Optimization of the U parameter in CoO groupings in ZnO (1010) and (1120) surfaces: a DFT+U and UPS study[1] KYLE STOLTZ, MARIO BORUNDA, Oklahoma State University-Stillwater — Cobalt oxide groupings in ZnO surface structures were studied using density functional theory within the Hubbard-like U (DFT+U) formalism to calculate the total energy of several configurations of this system. We find the U parameter by fitting the calculated density of states (DOS) to ultraviolet photoelectron spectroscopy measurements of pristine and doped ZnO nanostructures. It was found that the most energetically favorable configuration in the Co-doped ZnO nanostructures are clusters of CoO.

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