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First principles study of coulombic correlation effect on lithium doped zinc oxide nanocrystals[1] HYUNWOOK KWAK, MURILO L. TIAGO, University of Minnesota, JAMES R. CHELIKOWSKY, University of Texas — We examine the role of quantum confinement for impurities in zinc oxide nanocrystals. The electronic gap between the highest occupied level and the lowest unoccupied level for these systems will be larger than the band gap of bulk ZnO crystal owing to quantum confinement. We also expect quantum confinement to enhance correlation effects from on-site coulombic interactions, which will occur for lithium doped zinc oxide nanocrystals. We investigate the ionization energy for lithium impurities in ZnO nanocrystals and characterize the properties of the impurity levels. We assess the validity of arguments from recent experimental studies in which lithium impurities are expected to form shallow donors and acceptors in ZnO. We use a real-space ab initio pseudopotential method to obtain the ground state properties of an isolated nanocrystal. We use a rotationally invariant "LDA+U" scheme to model the on-site coulombic interaction of the zinc d-levels. The Hubbard U potential is rescaled for each nanocrystal using the static dielectric constant to reflect the reduced screening in a nanocrystal.

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