**Computational study of strain effect on the electronic properties of Cu-doped CdSe nanoplatelets**

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Colloidal Copper-doped nanocrystals(NCs) such as CdSe and PbS NCs is appealing due to their unique luminescence properties which are kwon to broad and tunable photoluminescence(PL) via charge-transfer recombination of conduction band electrons with copper localized holes. [1] However, to the best of our knowledge, Cu-doped Nanoplatelets(NPLs) colloidal system have not been systemically studied yet. Herein, by means of density functional theory (DFT) calculation, we investigate the ground-states and excited-states geometry and electronic properties of Cu+- and Cu2+-doped CdSe NPLs at the atomic level. In particular, we focus on the strain effect on the electronic properties of Cu+- and Cu2+-doped CdSe NPL capped with oleic acid organic ligand because colloidal CdSe NPLs, experimentally, can be stressed by self-scrolled via crystal growth. Our results showed that strain affects excited-state nuclear reorganization, which is responsible for broad PL shape and large PL stokes shift. We also computationally examined singlet and triplet excited-states configuration. These calculations yield fundamental perspectives to understand strain effect on electronic structure and photophysical properties of Cu-doped NPLs.

[1] H. D. Nelson, S. O. M. Hinterding, R. Fainblat, S. E. Creutz, X. Li, and D. R. Gamelin, J. Am. Chem. Soc. **139**, 6411 (2017).