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Characterizing the structural properties of organic-inorganic hybrid semiconductors by first-principles calculations CHANG-YOUN MOON, GUSTAVO DALPIAN, YONG ZHANG, SU-HUAI WEI, National Renewable Energy Laboratory, XIAOYING HUANG, JING LI, Department of Chemistry and Chemical Biology, Rutgers University — Recently, a new type of hybrid materials $A_{II}B_{VI}(en)_{0.5}$, consisting inorganic II-VI semiconductor slabs connected by organic molecule spacers have been synthesized.[1] These materials have the advantage of possessing both inorganic and organic constituents: good electric and optical properties of the inorganic part, and the easiness of assembly of the organic part.[1,2] In this work, using first principles method, we study the stability and structural properties of $A_{II}B_{VI}(en)_{0.5}$ (A=Zn or Cd, B=S, Se, or Te, and en=ethylenediamine) in the known α and β phases. We found that the relative stability of the α and β phases of the hybrids is closely related to the intrinsic stability of the two phases of the inorganic semiconductor constituent: wurtzite (WZ) and zincblende (ZB). An inorganic compound with WZ ground state will prefer to exist in the α phase, whereas a ZB compound will prefer to exist in the β phase.The relative stability is also affected by the size of the inorganic constituents and the spacing and bond angle of the en molecules. The results are analyzed by considering the contribution from the organic and inorganic part separately. [1] X. Huang et al., J. Am. Chem. Soc. 122, 8789 (2000); 125, 7049 (2003). [2] B. Fluegel et al., Phys. Rev. B 70, 205308 (2004)

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