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Fully Ordered and Nano-Structured Inorganic-Organic Hybrid Semiconductors YONG ZHANG, G. M. DALPIAN, B. FLUEGEL, S.-H. WEI, A. MASCARENHAS, National Renewable Energy Laboratory, X.-Y. HUANG, J. LI, Department of Chemistry, Rutgers University, NREL TEAM, RUTGERS TEAM — A family of novel inorganic-organic hybrid nanostructures based on II-VI semiconductors has been synthesized, including the first monolayer inorganic/organic superlattices with all covelent bonds (3D structures) and the smallest quantum wires (1D), the chains being formed of single II-VI atomic bonds [1]. These materials are atomistically reassembled crystals without the structural fluctuation typically found in other nanostrutures, and exhibit a number of remarkable properties (e.g., a giant bandgap tunability of 1-2 eV [1,2]). As a prototype system, a 3D structure β-ZnTe(en)$_{0.5}$ shows a strongly enhanced free exciton absorption (a few times of that in the II-VI binary), Raman lines as sharp as any binary semiconductor, band edge free exciton emission, and more than 10 times enhancement in the exciton binding energy. First-principles density function band structure calculations have been performed to obtain the band gap shift, dispersion relations (effective masses), and dielectric constants of the hybrid material, and the relevant band offsets. [1] X.-Y. Huang, J. Li, Y. Zhang, and A. Mascarenahs, JACS 125, 7049 (2003). [2] B. Fluegel, Y. Zhang, A. Mascarenahs, X.-Y. Huang, and J. Li, PRB 70, 205308 (2004).

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