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Structural and Electronic Properties of IV-VI Semiconductor Nanodots ROMAN LEITSMANN, FRIEDHELM BECHSTEDT, Institut für Festkörpertheorie und -optik, Friedrich-Schiller Universität Jena — The characterization of nanostructure properties versus dimension and surface passivation is of increasing importance for the nanotechnology. Especially the stoichiometry, geometry, and the electronic states of IV-VI semiconductor nanodots are of special interest [1,2]. We use ab initio methods to calculate structural and electronic properties of colloidal IV-VI semiconductor nanodots as a function of the dot diameter. A method to passivate the non-directional dangling bonds at the nanodot surfaces is derived and used to study the confinement effect on the HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) states. In addition we take the influence of relativistic (spin-orbit coupling – SOC) and excitonic effects into account. While the SOC leads to a considerable decrease of the HOMO-LUMO gap, excitonic effects play a minor role. [1] JACS 128, 10337 (2006) [2] JACS 129, 11354 (2007)

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