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Anomalous Photoluminescence in CdSe Quantum Dot Solids at High Pressure due to Non-uniform Stress. SEBASTIEN HAMEL, CHRISTIAN GRANT, JONATHAN CROWHURST, ANDREW WILLIAMSON, NATHALIA ZAITSEVA, Lawrence Livermore National Laboratory — The application of static high pressure provides a means to precisely control and investigate many fundamental and unique nanoparticle properties. CdSe is a model quantum dot (QD) system whose behavior under high pressure has been extensively studied; however, the effect of non-uniform stresses on this system has not been fully appreciated. In order to model these experiments and account for the behavior of the photoluminescence we carried out electronic structure simulations of wurtzite CdSe QDs with a core diameter of 2 to 5 nm using the Semi-Empirical Pseudopotential Method (SEPM). These calculations guide the interpretation of the photoluminescence data obtained from CdSe QD solids in different stress environments varying from purely uniform to highly non-uniform. Small deviations from a uniform stress distribution are found to profoundly affect the electronic properties of this system. In non-uniform stress environments, we observe a pronounced photoluminescence energy flattening above 3 GPa. The importance of this effect must be considered when investigating other potentially pressure mediated phenomena.

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