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First-principles Investigation of CdSe Nanowires using Wannier functions: Effects of Surface and Confinement on dielectric properties YOSUKE KANAI, Condensed Matter and Materials Division, Lawrence Livermore National Laboratory, JEFFREY GROSSMAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology, GIANCARLO CI-CERO, Materials Science and Chemical Engineering Department, Politecnico of Torino, Italy — Understanding how the electronic properties of a material change at the nanoscale is important for a wide range of technological applications as well as for basic science. One-dimensional nano-structures such as nanowires hold great promise for their potential application in opto-electronic devices. In this work, we investigate the electronic polarity behavior and transverse polarizability of hexagonal Cadmium Selenide (CdSe) nanowires of up to 3 nm in diameter, using a Wannier function description from density functional theory calculations. We address effects of quantum confinement and surfactant molecules on these nanowire properties via a local property analysis using the Wannier functions, revealing a few interesting insights in terms of local polarity changes. Interestingly, the transverse polarizability is enhanced and deviates significantly from the classical model for a dielectric cylinder at this scale. We will discuss our observation in terms of surface and confinement effects.

> Yosuke Kanai Condensed Matter and Materials Division, Lawrence Livermore National Laboratory

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