Exitonic Effects and Optical Absorption of the Silicon Nanowire

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We study electronic structure and optical absorption including excitonic effects in Hydrogen-passivated Silicon nanowire (SiNW) along [110] direction with first-principles calculation. In this work, Kohn-Sham equation, GW approximation and Bethe-Salpeter equation (BSE) are solved in plane wave space with ab initio pseudopotential. Due to the quantum confinement effect, the reduced screening interaction results in a large exciton bounding energy (1 eV). In addtion, the confined excitons cntribute to the optical absorption spectra by not only shifting the spectra but also enhancing some strong absorption peaks. Those strong peaks give rise to measure them in experiment. Focus on the exciton states, we observed Hydrogen-like excitons, and find their bounding energy are well discribed by 1-dimentional screening Coulomb interaction.