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Excitonic Effects and the Optical Properties of Silicon Nanowires[1]

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Semiconductor nanowires have potential applications in many fields such as optoelectronics, photovoltaic cells, and especially device miniaturization. The excited-state properties are of critical importance in the design of these functional devices. The low dimensionality and reduced size tend to strengthen the effective Coulomb interaction in these nanostructures. In this study, we focus on the correlated electron-hole states in semiconductor nanowires and the influence of this excitonic effect on the optical absorption spectra. First-principles calculations are performed for a hydrogen-passivated silicon nanowire of a diameter of 1.2 nm. Using plane waves and pseudopotentials, the quasiparticle states are calculated within the many-body perturbation theory with the so-called GW approximation. It is found that the fundamental gap depends on both the orientation and size of the wire, and that the gap increases as the diameter decreases in an inverse quadratic fashion [1]. The electron-hole interaction is then evaluated by the Bethe-Salpeter equation (BSE). The enhanced Coulomb interaction in this confined geometry not only gives rise to an unusually large exciton binding energy of more than 1 eV (compared to a value of 14.7 meV in silicon bulk), but also significantly modifies the relative strength of the absorption peaks. The characteristics of these exciton states will be discussed.
[1] "Quantum Confinement and Electronic Properties of Silicon Nanowires," X. Zhao, C. M. Wei, L. Yang, and M. Y. Chou, Phys. Rev. Lett. 92, 236805 (2004).

[1] In collaboration with Li Yang, Catalin D. Spataru, and Steven G. Louie