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Ab-initio calculations of optical spectra of silicon nanowires[1]
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— We present ab-initio calculations of absorption spectra of thin silicon nanowires (1-2 nm in diameter) and compare the results of different techniques. In particular we aim at assessing the ability of time dependent Density Functional Theory (TDDFT) to describe trends in the electronic properties of Si nanowires, by comparing results obtained within TDDFT with those of the Bethe-Salpeter Equation (BSE). We also discuss the numerical accuracy of both TDDFT and BSE calculations and the influence on computed spectra of several numerical parameters entering the calculations.

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