

Abstract Submitted
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Ab-initio calculations of absorption spectra of nanowires by solving the Bethe-Salpeter Equation¹ YUAN PING, DARIO ROCCA, Department of Chemistry, University of California, Davis, DEYU LU, Brookhaven National Laboratory, GIULIA GALLI, Department of Chemistry and Department of Physics, University of California, Davis — A first principle approach to the solution of the Bethe Salpeter equation without empty electronic states has been recently developed [1], which makes possible the calculations of absorption spectra of relatively large systems (with several hundreds of electrons). We present applications of this approach to quasi-one dimensional systems, including chains of hydrogen molecules and Si nanowires. We discuss techniques to further improve the performance of absorption spectra calculations, and present a general scheme to accurately integrate the divergence in the screened exchange integrals. Finally, in the case of Si nanowires, we discuss the effect of surface reconstruction in shaping optical absorption spectra.

[1] D. Rocca, D. Lu and G. Galli, J. Chem. Phys. 133, 164109 (2010)

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Yuan Ping
Department of Chemistry, University of California, Davis

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