

Abstract Submitted
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Ab-initio calculations of absorption spectra of Si nanostructures using iterative techniques to solve the Bethe-Salpeter Equation¹ YUAN PING, DARIO ROCCA, DEYU LU, Department of Chemistry, University of California, Davis, GIULIA GALLI, Department of Chemistry and Department of Physics, University of California, Davis — A first principle approach to solve the Bethe Salpeter equation has been recently proposed [1], that does not require the calculation of excited single particle orbitals, and thus opens the way to calculations of absorption spectra of relatively large systems. We show that the efficiency of this approach can be further improved: (i) by exploiting localization properties of the eigenvectors of the dielectric matrix entering the expression of the screened Coulomb interaction; and (ii) by adopting appropriate truncation schemes that allows one to accurately describe the dielectric matrix [2] with a small number of eigenvectors and eigenvalues . Applications to the calculation of absorption spectra of semiconducting clusters and Si nanorods will be presented. [1]D.Rocca, D.Lu and G.galli (submitted) [2]H.Wilson, F.Gygi and G.Galli, Phys. Rev. B 78, 113303 (2008); and H. Wilson, D. Lu, F. Gygi and G. Galli, Phys. Rev. B, 79, 245106, 2009.

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