Abstract Submitted
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Efficient evaluation of dielectric response functions and calculations of ground and excited state properties beyond local Density Functional approaches DEYU LU, Department of Chemistry, UC Davis, YAN LI, DARIO ROCCA, H. VIET NGUYEN, FRANCOIS GYGI, GIULIA GALLI — A recently developed technique to diagonalize iteratively dielectric matrices [1], is used to carry out efficient, ab-initio calculations of dispersion interactions, and excited state properties of nanostructures. In particular, we present results for the binding energies of weakly bonded molecular crystals [2], obtained at the EXX/RPA level of theory, and for absorption spectra of semiconducting clusters, obtained by an iterative solution of the Bethe-Salpeter equations [3]. We show that the ability to obtain the eigenmodes of dielectric matrices from Density Functional perturbation theory, without computing single particle excited states, greatly improves the efficiency of both EXX/RPA and many body perturbation theory [3,4] calculations and opens the way to large scale computations. [1] 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. [2] D. Lu, Y. Li, D. Rocca and G. Galli, Phys. Rev. Lett, 102, 206411, 2009; and Y. Li, D. Lu, V. Nguyen and G. Galli, J. Phys. Chem. C (submitted) [3] D. Rocca, D. Lu and G. Galli, submitted. [4] D. Lu, F. Gygi and G. Galli, Phys. Rev. Lett. 100, 147601, 2008. Work was funded by DOE/Scidac DE-FC02-06ER25794 and DOE/BES DE-FG02-06ER46262.

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