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Solution of the Bethe-Salpeter equation without empty electronic states: Applications to solids, nanostructures and molecules[1] DARIO ROCCA, YUAN PING, UC Davis, DEYU LU, Brookhaven National Laboratory, GIULIA GALLI, UC Davis — A method to solve the Bethe-Salpeter equation that avoids the explicit calculation of empty electronic states and the storage and inversion of dielectric matrices has been recently introduced [1-3]. This approach is suitable to compute the absorption spectra of large systems in a wide energy range and without relying on the Tamm-Dancoff approximation. We show the accuracy and scalability of this method by presenting calculations of absorption spectra of solids, molecules and nanostructures, including Si quantum dots and nanowires. In the case of nanowires, we discuss the influence of size and surface reconstruction on the optical properties.

[1] D. Rocca, D. Lu, and G. Galli, J. Chem. Phys. 133, 164109 (2010)
[2] D. Rocca, Y. Ping, R. Gebauer, and G. Galli, submitted to PRB
[3] Y. Ping, D. Rocca, D. Lu, and G. Galli, submitted to PRB

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