Abstract Submitted
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Opto-electronic properties of silicon nanoparticles: Excitation energies, sum rules, and Tamm-Dancoff approximation[1] MARTON VOROS, Physics Department, University of California, Davis, DARIO ROCCA, Université de Lorraine and CNRS, Nancy, ADAM GALI, Wigner Research Center for Physics, HAS, Budapest, GIULIA GALLI, The University of Chicago — We present an ab initio study of the excited state properties of silicon nanoparticles (NPs) with diameters of 1.2 and 1.6 nm. Quasiparticle corrections were computed within the GW approximation. The absorption spectra were computed by time-dependent density functional theory (TDDFT) using the adiabatic PBE approximation, and by solving the Bethe-Salpeter equation (BSE). In our calculations we used recently developed accelerated methods that avoid the explicit inversion of the dielectric matrix and summations over empty states [1]. We found that the scissor approximation reliably describes quasiparticle corrections for states in the low energy part of the spectra. We also found good agreement between the structure and positions of the absorption peaks obtained using TDDFT and the BSE. We discuss the effect of the Tamm-Dancoff approximation on the optical properties of the NPs and present a quantitative analysis in terms of sum rules. In the case of the BSE we found that, even in the absence of the Tamm-Dancoff approximation, the f-sum rule is not fully satisfied due to the inconsistency between the approximations used for the BSE kernel and for the quasiparticle Hamiltonian. [1] D. Rocca, D. Lu,G. Galli, J. Chem. Phys. 133, 164109 (2010).

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