Abstract Submitted
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Efficient calculation of optical linear response of large silicon clusters. GEFEI CHANG, University of Illinois at Urbana-Champaign, YIA-CHUNG CHANG, University of Illinois at Urbana-Champaign — Nanoscale silicon clusters have potential applications as light-emitting devices and bio-sensors. Ab initio calculations of the optical linear response of small-size nanoparticles have been performed via time-dependent density functional theory (TDDFT)[1] and by solving many-body Bethe-Salpeter equations (MBSE)[2,3]. We show that the ab initio calculations can be made much more efficient when the nanocluster possess high point group symmetry and symmetrized basis functions are used. This allows us to extend the ab initio calculation to much larger Si clusters (up to a few hundred Si atoms) on a personal computer. The optical linear response of Si nanocluster (passivated with hydrogen) as a function of cluster size is examined. The effect of phosphorus doping of Si nanocluster on its optical properties is also studied.

1. O$\hat{g}$ũt,S., J. R. Chelikowsky, and S. G. Louie, PRL 80, 3162(1998); Marques, M., A. Castro, and A. Rubio, J. Chem. Phys. 115, 3006(2001). 2. Rohlfing, M., and S. G. Louie, PRL 80, 3320(1998);PRB 62, 4927(2000). 3. Grossman, J. C., M. Rohlfing, L. Mitas, S. G. Louie, and M. L. Cohen,PRL 86, 472(2001).

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