

Efficient algorithms for the electronic structure of nanocrystals

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We present a subspace iteration method to solve the self-consistent Kohn-Sham eigenvalue problem. Instead of computing eigenvectors explicitly for each self-consistent-field iteration, the occupied eigen subspace is progressively optimized by damped Chebyshev polynomial filtering¹. The number of iterations is similar to an eigensolver-based approach; however, the subspace iteration can be over an order of magnitude faster than direct diagonalization. With a real space grid and pseudopotential approach, we will illustrate the method for P-doped Si nanocrystals up to 6 nm in diameter² (over 5,000 atoms). Our calculated size dependence of hyperfine splitting is in excellent agreement with experimental data. We also examined the evolution of the defect wave function and its binding energy with nanocrystal size.

- [1] Y. Zhou, Y. Saad, M. L. Tiago, and J. R. Chelikowsky, *J. Comp. Phys.*, **219**, 172 (2006).
- [2] T.-L. Chan, M. L. Tiago, E. Kaxiras, and J. R. Chelikowsky, *Nano Letters* **8**, 596 (2008).