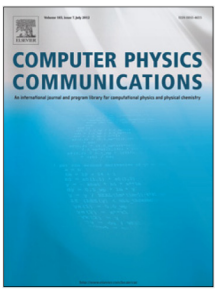
Accepted Manuscript



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D. Gabay, X. Wang, V. Lomakin, A. Boag, M. Jain, A. Natan

PII: S0010-4655(17)30248-5
DOI: http://dx.doi.org/10.1016/j.cpc.2017.08.005
Reference: COMPHY 6288

To appear in: *Computer Physics Communications*

Received date : 11 July 2017
Accepted date : 2 August 2017

Please cite this article as: D. Gabay, X. Wang, V. Lomakin, A. Boag, M. Jain, A. Natan, Size dependent electronic properties of silicon quantum dots—An analysis with hybrid, screened hybrid and local density functional theory, *Computer Physics Communications* (2017), http://dx.doi.org/10.1016/j.cpc.2017.08.005

Size dependent electronic properties of silicon quantum dots - an analysis with hybrid, screened hybrid and local density functional theory

D. Gabay[a], X. Wang[b], V. Lomakin[b], A. Boag[a], M. Jain[c], A. Natan[a,d,*]

[a]*Department of Physical Electronics, Tel-Aviv University, Tel-Aviv, Israel 69978*
[b]*Department of Electrical and Computer Engineering, University of California, San Diego, La Jolla, CA 92093, USA*
[c]*Department of Physics, Indian Institute of Science, Bangalore 560 012, India*
[d]*The Sackler center for computational molecular and materials science, Tel-Aviv University, Tel-Aviv, Israel 69978*

Abstract

We use an efficient projection scheme for the Fock operator to analyze the size dependence of silicon quantum dots (QDs) electronic properties. We compare the behavior of hybrid, screened hybrid and local density functionals as a function of the dot size up to ∼800 silicon atoms and volume of up to ∼20nm^3. This allows comparing the calculations of hybrid and screened hybrid functionals to experimental results over a wide range of QD sizes. We demonstrate the size dependent behavior of the band gap, density of states, ionization potential and HOMO level shift after ionization. We also demonstrate how the use of Graphical Processing Units (GPUs) can accelerate further such calculations.

1. Introduction

Quantum dots (QDs) form a class of nanometer scale materials that present an efficient way to tune the electronic and optical properties of materials by controlling their size [1, 2, 3]. In particular, the optical band gap and electronic density of states are affected by quantum confinement effects [1, 2, 3]. Silicon based QDs are especially interesting as silicon is a highly abundant element with a wide use in electronics, photovoltaics, and many other fields. They were therefore the subject of both experimental [4, 5, 6, 7, 8, 9] and theoretical [10, 11, 12, 13, 8, 9, 14, 15] research.

Even a small QD can have hundreds of atoms and hence present a challenge for full quantum calculations. Semi-empirical quantum methods such as tight-binding [16] (TB)