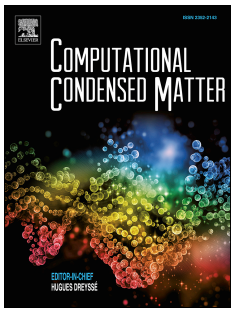
Accepted Manuscript



Structural and electronic properties of silicon carbide polytypes as predicted by exact exchange calculations

N. Gonzalez Szwacki

PII: S2352-2143(17)30062-X

DOI: 10.1016/j.cocom.2017.09.003

Reference: COCOM 93

To appear in: *Computational Condensed Matter*

Received Date: 21 March 2017

Revised Date: 16 August 2017

Accepted Date: 15 September 2017

Please cite this article as: N.G. Szwacki, Structural and electronic properties of silicon carbide polytypes as predicted by exact exchange calculations, *Computational Condensed Matter* (2017), doi: 10.1016/j.cocom.2017.09.003.

Structural and electronic properties of silicon carbide polytypes as predicted by exact exchange calculations

N. Gonzalez Szwacki

Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, ul. Pasteura 5, PL-02-093 Warsaw, Poland

Abstract

A full-potential band structure calculation within the exact exchange-optimized effective potential (EXX-OEP) approach was performed for the 3C, 6H, 15R, 4H, and 2H polytypes of SiC. The calculated lattice constants and energy band gaps were found to be in a good agreement with experimental values; therefore, the EXX-OEP method, although computationally expensive, is a viable method for solving the long-standing band gap problem of density functional theory (DFT). Throughout the paper, the results obtained using EXX-OEP are compared with those obtained using regular DFT calculations.

Keywords: silicon carbide, semiconductors, lattice parameters, electronic structure, EXX-OEP approach

1. Introduction

The exact exchange (EXX) method, which uses the Fock term calculated on the Kohn-Sham orbitals, provides a method to extend the traditional density functional theory (DFT) formalism, which employs approximate exchange-correlation functionals. Since the Fock term depends on the density only implicitly via the Kohn-Sham orbitals, $\phi_i[n]$, the functional derivative of the exchange-correlation energy, E_{xc}, that is $\delta E_{xc}/\delta n = u_{xc}$, cannot be calculated directly. Instead, indirect approaches must be used to minimize the total energy functional,

*Corresponding author
Email address: gonz@fuw.edu.pl (N. Gonzalez Szwacki)