

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](https://doi.org/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.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

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-
5 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)

Download English Version:

<https://daneshyari.com/en/article/7956761>

Download Persian Version:

<https://daneshyari.com/article/7956761>

[Daneshyari.com](https://daneshyari.com)