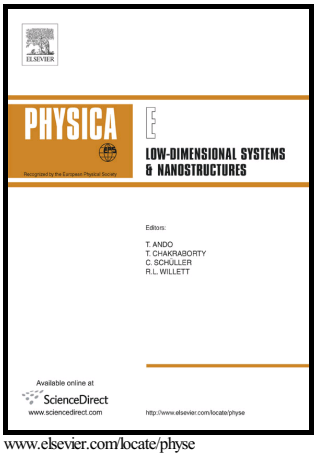
Author's Accepted Manuscript



www.elsevier.com/locate/physe

Optical properties of geometrically optimized graphene quantum dots

Paweł Bugajny, Ludmiła Szulakowska, Błazej Jaworowski, Paweł Potasz

PII: S1386-9477(16)30390-3
DOI: http://dx.doi.org/10.1016/j.physe.2016.08.030
Reference: PHYSE12563

To appear in: *Physica E: Low-dimensional Systems and Nanostructures*

Received date: 12 May 2016
Revised date: 20 August 2016
Accepted date: 29 August 2016

Cite this article as: Paweł Bugajny, Ludmiła Szulakowska, Błazej Jaworowsk and Paweł Potasz, Optical properties of geometrically optimized graphen quantum dots, *Physica E: Low-dimensional Systems and Nanostructures* http://dx.doi.org/10.1016/j.physe.2016.08.030

Optical properties of geometrically optimized graphene quantum dots

Paweł Bugajny[1], Ludmiła Szulakowska[2], Błazej Jaworowski[1], Paweł Potasz[1]

[1] *Department of Theoretical Physics, Wroclaw University of Technology, Wybrzeze Wyspianskiego 27, 50-370 Wroclaw, Poland*
[2] *Department of Physics, Advanced Research Complex, 25 Templeton Str.,University of Ottawa, Ottawa, Ontario, K1N 6N5, Canada*

Abstract

We derive effective tight-binding model for geometrically optimized graphene quantum dots and based on it we investigate corresponding changes in their optical properties in comparison to ideal structures. We consider hexagonal and triangular dots with zigzag and armchair edges. Using density functional theory methods we show that displacement of lattice sites leads to changes in atomic distances and in consequence modifies their energy spectrum. We derive appropriate model within tight-binding method with edge-modified hopping integrals. Using group theoretical analyzis, we determine allowed optical transitions and investigate oscillatory strength between bulk-bulk, bulk-edge and edge-edge transitions. We compare optical joint density of states for ideal and geometry optimized structures. We also investigate an enhanced effect of sites displacement which can be designed in artificial graphene-like nanostructures. A shift of absorption peaks is found for small structures, vanishing with increasing system size.

Keywords: `graphene quantum dots, optical properties`

1. Introduction

Graphene quantum dots (GQDs) reveal many peculiar electronic properties that are shape- and edge-dependent, which makes them promising candidates for building blocks of the future opto-electronic devices [1, 2, 3]. Within possible