10 years of research and education network Linköping University – Federal University of Bahia

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October 2018



LiU - UFBA network Leadership

Assoc. Prof. Gueorgui K. Gueorguiev, LiU



Dr. G. K. Gueorguiev completed his *PhD* on the structural and electronic properties of carbon- and silicon-based clusters in 2003 at Coimbra University, Portugal, with the exceptional mark "Cum Laude" and following a fellowship from the prestigious Portuguese Instituto Camões. He is project and research leader (VR, SSF) focusing on the design of nanostructured carbon-based thin films with pre-defined properties and with experimental verification. He is the initiator and leader of the network between LiU and UFBA (STINT, VR-SRL) operating for more than 10 years, generating excellent results in research and education. His research interests expand towards 2D and van der Waals structures (WP leader in FLAG-ERA GRIFONE), and layered compounds. Theoretical approaches include first-principles and effective methods in computational materials science, synthesis techniques involve magnetron sputtering, metal-organic-CVD, atomic-layer deposition.

Assoc. Prof. Roberto Rivelino, UFBA



Dr. R. Rivelino, Background and research interests: Electronic structure methods combined with advanced scientific computing have changed our capacity to perform molecular modeling and simulation studies of fundamental processes in condensed matter physics, chemistry, nanoscience, and biology. These methods provide realistic results with full atomic resolution. Our research efforts are focused on advancing this emerging capability and applying it to important problems in physics and chemistry. For example, we are currently investigating electron transport through low-dimensional materials aiming at efficient nanodevices for spintronic applications. Additionally, we are employing atomistic simulations to investigate finite-temperature dynamics of chemical systems in solution and proton-transfer in biomolecules adsorbed onto metallic or semiconducting surfaces. Using these theoretical approaches, we hope to contribute to the development of theoretical chemistry as well as to boost new experiments in this area of research.

Assoc. Prof. Anelia Kakanakova, LiU



Dr. A. Kakanakova, Expanding a platform for groundbreaking materials in group III nitrides of both scientific and technological relevance derived by metal organic chemical vapor deposition (MOCVD). She has attracted prestigious grants from the Swedish Research Council (VR), and The Sweden's Innovation Agency (VINNOVA), including : 2002 VR Junior Researcher Position Grant; 2008 VR University Lecturer Position Grant; 2011 VINNOVA VINNMER Fellowship Grant with The Cambridge Centre for Gallium Nitride, University of Cambridge, UK. Her present focus is on the development of emerging graphitic-like group III nitrides (PI and Coordinator of FLAG-ERA JTC project GRIFONE in synergy with the FET Graphene Flagship).

Abstract

- In *10 years*, we have built-up *strong and competitive research and education network in material science* between *Linköping University* (*LiU*) and *Federal University of Bahia* (*UFBA*) involving more than 15 members from both research teams with breakthrough achievements in several different hot-topic research lines in materials science, joint supervision of PhD students, exchange research visits and high-level of jointly organized events and excellence seminars
- We promoted Agreement on Academic, Cultural, and Scientific Cooperation between Federal University of Bahia, Salvador, Brazil, and Linköping University, Sweden:
 - Signed 23 March 2016 by

Prof. João Carlos Salles Pires da Silva, Rector of UFBA and Prof. Peter Värbrand, Vice President of Linköping University

- Currently, *our network is expanding* by involving excellent research teams from other universities in Brazil including
 - University of São Paulo, Federal University of Paraná, Federal University of São Carlos and Federal University of Santa Maria



Joint Projects



STINT The Swedish Foundation for International Cooperation in Research and Higher Education

- Joint Project (1): STINT 2009-2014
 - > Type of grant: *Institutional Grant for younger researchers*
 - Title: Developing a flexible theoretical approach for designing inherently nanostructured and cluster-assembled materials
 - Main applicants: Gueorgui K. Gueorguiev, LiU and Roberto Rivelino de M. Moreno, UFBA
- Joint Project (2): CAPES 2012-2015
 - Type of grant: PDSE scholarships: program for shared PhD between Brazilian and foreign partner
 - Title: Multiscale design of low-dimensional materials for applications in optical nano-devices and nano-electronics
 - Main applicants: Roberto Rivelino de M. Moreno, UFBA;
 Gueorgui K. Gueorguiev, LiU; Fernando de Brito Mota, UFBA; and
 Caio M. de Castilho, UFBA
 - > Three scholarships to:
 - > Maria Isabel Oliveira, recruited at LiU for 12 months
 - > *Renato Batista dos Santos*, recruited at LiU for 18 months
 - > Rafael Rodrigues de Queiroz Freitas , recruited at LiU for 16 months





Joint Projects

- Joint Project (3): Swedish Research Council (VR) 2014-2018
 - > Type of grant: *Research Grant*
 - > Title: Steering AlN as a modern-technology-relevant semiconductor material
 - Main applicant: Anelia Kakanakova, LiU and Co-applicant: Fernando de Brito Mota, UFBA
- Joint Project (4): Swedish Research Council (VR) 2015-2018
 - > Type of grant: *Swedish Research Links*
 - Title: Multiscale design of low-dimensional materials for applications in optical nano-devices and nano-electronics
 - Main applicants: Gueorgui K. Gueorguiev, LiU and Roberto Rivelino de M. Moreno, UFBA
- Joint Project (5): CNPq 2015-2018
 - > Type of grant: *Research Fellowship*
 - > Title: Computer simulations for low-dimensional materials
 - > Main applicant: Roberto Rivelino de M. Moreno, UFBA







Hot topics research in materials science

- > More than 20 joint scientific articles
- > More than 10 presentations at major international conferences



Low-dimensional carbon-based systems



PHYSICAL REVIEW B 84, 075417 (2011)

Effects of N doping on the electronic properties of a small carbon atomic chain with distinct sp^2 terminations: A first-principles study

Renato B. dos Santos,^{1,*} R. Rivelino,^{1,†} F. de Brito Mota,¹ and G. K. Gueorguiev^{2,‡}

THE JOURNAL OF PHYSICAL CHEMISTRY C

THE JOURNAL OF PHYSICAL CHEMISTRY

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Article

Article pubs.acs.org/JPCA

Electric-Field Control of Spin-Polarization and Semiconductor-to-Metal Transition in Carbon-Atom-Chain Devices

Renato Batista dos Santos,^{†,§} Fernando de Brito Mota,[†] Roberto Rivelino,^{**†} and Gueorgui K. Gueorguiev**



Emerging 2D group III nitrides

Eur. Phys. J. B (2012) 85: 48 DOI: 10.1140/epjb/e2011-20538-6

Regular Article

THE EUROPEAN PHYSICAL JOURNAL B

Defects in hexagonal-AIN sheets by first-principles calculations

E.F. de Almeida Junior¹, F. de Brito Mota^{1,a}, C.M.C. de Castilho^{1,2}, A. Kakanakova-Georgieva³, and G.K. Gueorguiev³





New knowledge to the rational deposition of (ultra)thin films of group III nitrides ⁹



Topological insulators and 2D group III bismides

THE JOURNAL OF PHYSICAL CHEMISTRY C Dubsacs.org/JPCC Topological Insulating Phases in Two-Dimensional Bismuthcontaining Single Layers Preserved by Hydrogenation Bismuth-Sill R. R. Q. Freitas, [†]&[‡] R. Rivelino,^{&†} F. de Brito Mota, ^{§,†} and C. M. C. de Castilho^{&,§,II} ^{*} ¹Instituto de Física, Universidade Federal da Bahia, 40170-115 Salvador, Bahia, Brazil [§]Gnpo de Física de Superficies e Materiais, Instituto de Física, Universidade Federal da Bahia, Campus Universitário da Federação, 40170-115 Salvador, Bahia, Brazil ^{II}Instituto Nacional de Ciência e Tecnologia em Energia e Ambiente (CIENAM) INCT-E&A, Universidade Federal da Bahia, 40170-280 Salvador, Bahia, Brazil A. Kakanakova-Georgieva[‡] and G. K. Gueorguiev[‡] ^{*}Department of Physics, Chemistry and Biology (IFM), Linköping University, 581 83 Linköping, Sweden



IOP Publishing Nanotechnology 27 (2016) 055704 (11pp)

doi:10.1088/0957-4484/27/5/055704

Nanotechnology

Tuning band inversion symmetry of buckled III-Bi sheets by halogenation

R R Q Freitas^{1,2}, F de Brito Mota¹, R Rivelino¹, C M C de Castilho^{1,3}, A Kakanakova-Georgieva² and G K Gueorguiev²

IOP Publishing J. Phys.: Condens. Matter 27 (2015) 485306 (8pp) Journal of Physics: Condensed Matter doi:10.1088/0953-8984/27/48/485306

Spin-orbit-induced gap modification in buckled honeycomb XBi and XBi_3 (X = B, AI, Ga, and In) sheets

R R Q Freitas^{1,2}, F de Brito Mota¹, R Rivelino¹, C M C de Castilho^{1,3}, A Kakanakova-Georgieva² and G K Gueorguiev²



Low-dimensional silicon boride systems





Si-based nanostructured materials

THE JOURNAL OF PHYSICAL CHEMISTRY C

Optical Properties and Quasiparticle Band Gaps of Transition-Metal Atoms Encapsulated by Silicon Cages

M. I. A. Oliveira,^{†,‡} R. Rivelino,^{*,†} F. de Brito Mota,[†] and G. K. Gueorguiev^{*,‡}

[†]Instituto de Física, Universidade Federal da Bahia, 40210-340 Salvador, Bahia, Brazil

[‡]Department of Physics, Chemistry and Biology (IFM), Linköping University, S-581 83 Linköping, Sweden

Supporting Information

ABSTRACT: Semiconductors assembled upon nanotemplates consisting of metal-encapsulating Si cage clusters ($M@Si_n$) have been proposed as prospective materials for nanodevices. To make an accurate and systematic prediction of the optical properties of such $M@Si_n$ clusters, which represent a new type of metal-silicon hybrid material for components in nanoelectronics, we have performed first-principles calculations of the electronic properties and quasiparticle band gaps for a variety of $M@Si_{12}$ (M = Ti, Cr, Zr, Mo, Ru, Pd, Hf, and Os) and $M@Si_{16}$ (M = Ti, Cr, and Hf) clusters. At first stage, the electronic structure calculations have been performed within plane-wave density functional theory in order to predict equilibrium geometries, polarizabilities, and optical absorption spectra of



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these endohedral cagelike clusters. The quasiparticle calculations were performed within the *GW* approximation, which predict that all of these systems are semiconductors exhibiting large band gaps. The present results have demonstrated that the independent-particle absorption spectra of $M@Si_n$, calculated within the local density or generalized gradient approximations to density functional theory, are dramatically influenced by many-body effects. On average, the quasiparticle band gaps were significantly increased, in comparison with the independent-particle gaps, giving values in the 2.45–5.64 eV range. Consequently, the inclusion of many-body effects in the electron–electron interaction, and going beyond the mean-field approximation of independent particles, might be essential to realistically describe the optical spectra of isolated $M@Si_n$ clusters, as well as their cluster-assembled materials.



Biomolecules adsorbed on metal surfaces





PhD students, senior researchers and exchange research visits

- > More than 30 exchange research visits
- > PhD courses at UFBA and LiU



- Dr. *Maria Isabel Almeida Oliveira*, UFBA-IFM, *Optical absorption of Silicon-based nanostructures: Ab initio simulations including many body effects by the GW approximation*, *defended 24 April 2014* (12 months at LiU)
- Dr. *Renato Batista dos Santos*, UFBA-IFM, *Ab initio study of low-dimensional materials: from one-dimesnional carbon chains to 2D systems similar to graphene*, *defended 18 December 2015* (18 months at LiU)
- Dr. *Rafael Rodriguês Freitas*, UFBA-IFM, *Structural, electronic and toplogical properties of 2D systems containing bismuth*, *defended 05 August 2016* (16 months at LiU)
- Dr. *Edward Almeida Jr.*, UFBA-IFM, *Theoretical studies of the structural and electronic properties od 2D materials based on hexagonal Aluminum Nitride (h-AlN)*, *defended 12 August 2016* (4 months at LiU)
- Dr. *Cecilia Goyenola*, IFM, *Nanostructured carbon-based thin films: prediction and design*, *defended 16 October 2015* (1 month at UFBA)
- Dr. *Paulo Medeiros*, IFM, *Electronic properties of complex interfaces and nanostructures*, *defended 05 June 2015* (Master student at UFBA, PhD student at LiU)



Jointly organized events and excellence seminars





Symposium: Beyond Graphene - Low-dimensional systems based on graphene and III-nitrides

Scope of the Symposium:

Tailored low-dimensional systems based on graphene and with the possibility of integrating other 2D networks, III-Nitrides included (AIN, BN, GaN, etc), become implicit part of perceived graphene-based applications. Specifically, III-Nitrides is a material system that, besides the low-dimensional systems understood as 2D networks, accommodates low-dimensional systems in the fashion of quantum wells in epitaxial structures for optoelectronic applications. An emerging aspect of the interconnection between graphene and III-Nitrides is related to the deposition of III-Nitrides epitaxial structures on graphene-based templates. The scope of the symposium is then to advance the knowledge on graphene-like structures, III-Nitrides and other 2D systems either as individual as well as complementary systems and also in the context of their various interconnections.

Abstracts will be solicited in (but not limited to) the following areas:

- Theoretical modeling of growth, structural evolution, controllable incorporation of defects and doping of graphene;
- Tailored low-dimensional carbon-based nano-units, nano-ribbons and nano-wires, including modeling, experimental growth and functionalization;
- Theoretical modeling of growth, structural evolution, controllable incorporation of defects and doping of 2D networks beyond graphene, including III-Nitrides;
- · Deposition of graphene and 2D networks beyond graphene;
- · Aspects of epitaxial growth of III-Nitrides: quantum well structures and graphene templates;
- Modeling of gas-phase chemistry, surface reactions and interfaces involved in the deposition on/of graphene and III-Nitrides and their assembly;
- · Electronic and mechanical properties of graphene, III-Nitrides and other 2D networks;
- · Excited state properties (optical and magnetic) of graphene, III-Nitrides and other 2D networks.

Symposium Organizers:

- 1. Prof. Caio M.C. de Castilho Universidade Federal da Bahia, UFBA, Brazil
- 2. Prof. Fernando de Brito Mota
- Universidade Federal da Bahia, UFBA, Brazil 3. Assoc. Prof. Gueorgui K. Gueorguiev
- Linköping University, Sweden 4. Assoc. Prof. Anelia Kakanakova-Georgieva
- Linköping University, Sweden





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- 1. Prof. Caio M.C. de Castilho Universidade Federal da Bahia, UFBA, Brazil
- 2. Prof. Fernando de Brito Mota Universidade Federal da Bahia, UFBA, Brazil
- 3. Assoc. Prof. Gueorgui K. Gueorguiev Linköping University, Sweden
- 4. Assoc. Prof. Anelia Kakanakova-Georgieva Linköping University, Sweden



The XIII SBPMat comprised of 19 Symposia involving topics as synthesis of new materials, computer simulations, carbon and graphene nanostructures, energy storage systems, surface engineering, innovation and technology transfer in materials research; and attracted more than 1000 participants

Anelia Kakanakova was Chair of a Plenary session





Session 2 Novel Functional Materials & Nanotechnology



Geurgui Guerguiev

Mail: gekos@ifm.liu.se Web: www.ifm.liu.se/materialphysics/ thinfilm/staff/gueorguigueorguiev/index.xml Position: Senior University Lecturer (Associate Professor) in Computational Material Science

University (or other affiliation): Linköping University

Title of presentation: Design of nanostructured and layered materials

Keywords: Carbon, silicon, thin films, layered materials, III-Nitrides, bismuthides, borides, DFT, CVD, magnetron sputtering

Background and research interests: Dr. Gueorguiev completed his PhD on the structural and electronic properties of carbon- and silicon-based clusters in 2003 at Coimbra University, Portugal, with the exceptional mark "Cum Laude" and following a fellowship from the prestigious Portuguese Instituto Camões. Presently, he is project- and research leader (VR, SSF) focusing on the design of nanostructured carbon-based thin films with pre-defined properties and with experimental verification. He is the initiator and leader of a scientific network between LiU and Federal University of Bahia (STINT, VR-SRL) operating for more than 7 years, involving 15 team members from both institutions and generating excellent research and education results (so far 5 Brazilian PhD students jointly supervised at long-term research visits at LiU). His research interests expand towards 2D and van der Waals structures (WP leader in FLAG-ERA GRIFONE), layered compounds. Theoretical approaches include first-principles and effective methods in computational materials science, synthesis techniques involve magnetron sputtering, metal-organic-CVD, atomic-layer deposition.

Position: PhD in Physics

University (or other affiliation): Federal University of Bahia

Title of presentation: What is so interesting and challenging in the flatland?

Keywords: Electronic structure, atomistic simulation, molecular spectroscopy, molecular modeling, topological insulator, optical properties

Background and research interests: Electronic structure methods combined with advanced scientific computing have changed our capacity to perform molecular modeling and simulation studies of fundamental processes in condensed matter physics, chemistry, nanoscience, and biology. These methods provide realistic results with full atomic resolution. Our research efforts are focused on advancing this emerging capability and applying it to important problems in physics and chemistry. For example, we are currently investigating electron transport through low-dimensional materials aiming at efficient nanodevices for spintronic applications. Additionally, we are employing atomistic simulations to investigate finite-temperature dynamics of chemical systems in solution and proton-transfer in biomolecules adsorbed onto metallic or semiconducting surfaces. Using these theoretical approaches, we hope to contribute to the development of theoretical chemistry as well as to boost new experiments in this area of research.



Roberto Rivelino de Melo Moreno

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HOME	HOME >
ENSINO	EVENTOS
PESQUISA	
OUTRAS ATIVIDADES	
CONTATO	Workshop on
@nanogrupo	2D and layered materials: from honeycomb sheets to nanocomposites
G+	11-13 April 2017 Catussaba Business, Salvador, Bahia, Brazil Organizers:
	Assoc. Prof. Gueorgui K. Gueorguiev (Chairman) Department of Physics, Chemistry and Biology (IFM), Linköping University(LiU), Linköping, Sweden;
	and
	Assoc, Prof. Roberto Rivelino (Vice-chairman) Instituto de Física, Universidade Federal da

The workshop was attended by researchers and students from Federal University of Bahia and Linköping University, but also by leading researchers from Federal University of Paraná, Federal University of São Carlos (São Paulo state), and Federal University of Santa Maria (Rio Grande do Sul state)







New research synergies

Recognition of the achievements of the LiU-UFBA network and its potential

