EUROPEAN CURRICULUM VITAE FORMAT

PERSONAL INFORMATION

Name	**FABRIZIO GALA**
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Telephone	
E-mail	**fabrizio.gala@uniroma1.it**
Nationality	Italian
Date of birth	11/03/1978

WORK EXPERIENCE

• Dates (from – to)	01/2013-12/2013
• Name and address of employer	Dipartimento S.B.A.I. (Scienze di Base e Applicate per l'Ingegneria) Sezione di Fisica – University of Rome "La Sapienza".
• Type of business or sector	Postdoctoral research in computational physics, "Tecniche numeriche di fisica computazionale su piattaforme GPU"
• Occupation or position held	postdoctoral research fellow
• Dates (from – to)	07/2008-12/2012
• Name and address of employer	Dipartimento S.B.A.I. (Scienze di Base e Applicate per l'Ingegneria) Sezione di Fisica – University of Rome "La Sapienza".
• Type of business or sector	Postdoctoral research in solid state physics, "Studio delle propietà elettroniche e vibrazionali di nano-strutture"
• Occupation or position held	postdoctoral research fellow
• Dates (from – to)	09/2006-02/2007
• Name and address of employer	Dipartimento di Energetica – University of Rome "La Sapienza".
• Type of business or sector	Postdoctoral research in computational physics, "Sviluppo di un codice scalabile linearmente di dinamica molecolare"
• Occupation or position held	postdoctoral research fellow

EDUCATION

• Dates (from – to)	2005-2008
• Name and type of organisation providing education and training	University of Rome "La Sapienza"
• Principal subjects/occupational skills covered	Electromagnetism and Materials Science, title of the phD thesis: "Structural and electronic properties of GaAs and Carbon based nano-structures."
• Title of qualification awarded	Philosophiae Doctor (phD) in ELECTROMAGNETISM
• Dates (from – to)	1997-2003
• Name and type of organisation providing education and training	University of Rome "La Sapienza"
• Principal subjects/occupational skills covered	Theoretical Physics, title of the master thesis: "Compressione di sequenze e mappe dell'intervallo [0,1] in sè".
• Title of qualification awarded	Master Degree in Physics

• Level in national classification	110/110 cum laude

COURSES AND TRAINING

• Dates (from – to)	18/10/2010-22/10/2010
• Name and type of organisation providing education and training	SISSA - International School for Advanced Studies, Trieste, Italy
• Course	NanoExcite Workshop 2010
• Title of qualification awarded	Certificate for successfully finished course
• Dates (from – to)	14/06/2010-18/06/2010
• Name and type of organisation providing education and training	CISM, International Centre for Mechanical Sciences, Energy and Environment, Fluid Mechanics, Udine, Italy
• Course	Nano- and Micro- Mechanics of Living Cell Adhesion
• Title of qualification awarded	Certificate for successfully finished course
• Dates (from – to)	13/11/2006-17/11/2006
• Name and type of organisation providing education and training	CECAM, Lyon, France
• Course	Simulating matter at the nano-scale using density-functional theory, pseudopotentials and plane waves
• Title of qualification awarded	Certificate for successfully finished course
• Dates (from – to)	04/07/2005-15/07/2005
• Name and type of organisation providing education and training	CINECA, Casalecchio di Reno (BO), Italy
• Course	XIV Summer School in Parallel Computing
• Title of qualification awarded	Certificate for successfully finished course

TEACHING EXPERIENCE

• Academic Year	2013-2014
• Laurea Degree Course	Corso di Laurea in Ingegneria, sede di Latina – University of Rome "La Sapienza".
• Lecture/Course	FISICA I (CF 3)
• Position held	Adjunct Professor
• Academic Year	2012-2013
• Laurea Degree Course	Corso di Laurea in Ingegneria Chimica – University of Rome "La Sapienza".
• Lecture/Course	FISICA II (CF 4)
• Position held	Adjunct Professor
• Academic Year	2011-2012
• Laurea Degree Course	Corso di Laurea in Ingegneria Meccanica – University of Rome "La Sapienza".
• Lecture/Course	FISICA I (CF 2)
• Position held	Adjunct Professor
• Academic Year	2010-2011
• Laurea Degree Course	Corso di Laurea in Ingegneria Meccanica – University of Rome "La Sapienza".
• Lecture/Course	LABORATORIO DI FISICA (CF 3)
• Position held	Adjunct Professor
• Academic Year	2009-2010 ; 2008-2009 ; 2007-2008
• Laurea Degree Course	Corso di Laurea in Ingegneria Meccanica – University of Rome "La Sapienza".
• Lecture/Course	FISICA 2
• Position held	Tutor

• Academic Year	2007-2008
• Laurea Degree Course	Corso di Laurea in Ingegneria Meccanica – University of Rome "La Sapienza".
• Lecture/Course	LABORATORIO DI FISICA
• Position held	Tutor
• Academic Year	2006-2007
• Laurea Degree Course	Corso di Laurea in Ingegneria Civile – University of Rome "La Sapienza".
• Lecture/Course	FISICA I
• Position held	Tutor
• Academic Year	2005-2006
• Laurea Degree Course	Corso di Laurea in Ingegneria Meccanica – University of Rome "La Sapienza".
• Lecture/Course	LABORATORIO DI FISICA
• Position held	Tutor

PERSONAL SKILLS AND COMPETENCES

MOTHER TONGUE	ITALIAN
OTHER LANGUAGES	
	ENGLISH
• Reading skills	EXCELLENT
• Writing skills	GOOD
• Verbal skills	GOOD
COMPUTER PROGRAMMING EXPERIENCE	Vast experience in several programming languages including Fortran90,C and C++, in the MPI paradigm for scientific parallel applications, as well as in CUDA programming.

RESEARCH ACTIVITIES

Stability properties of point and extended self-interstial defects in crystals of gallium arsenide (GaAs).

GaAs is a binary semiconductor compound extensively employed in industrial devices. Two different quantum mechanical simulation schemes have been used, such as total energy calculations from first principles, based on density functional theory (DFT), and the tight-binding molecular dynamics (TBMD), that is a good compromise between accuracy and computational workload, and which guarantees reliable predictions on nano-sized systems. On one hand the properties of ground-state interstitial complex structures (I_n) have been studied by means of semi-empirical tight-binding molecular dynamics, via an optimization procedure made of a simulated annealing up to a target temperature and a damped dynamics. Due to the complexity of the possible topology, reaction paths and stoichiometry, the analysis has been restricted to In with $n \leq 7$ that, anyway, has been shown to be sufficient to extrapolate some important conclusions concerning the growth process of extended defects in GaAs. On the other hand, the relative importance of I_1 and I_2 capture process have been clarified thorugh *ab initio* calculations of the diffusion activation energy of these two species, as any aggregation may actually take place only if these complexes are able to migrate rapidly through the lattice. Thus the migration paths and the capture/release processes of such complexes have been studied in detail from first principle calculations.

Methane adsorption on carbon based nano-structures, as single walled nanotubes (SWCNTs), or bundles of nanotubes.

The problem of physical and chemical adsorption of gaseous methane molecules on such structures, has been investigated, mainly because of its potential interest in applications for hydrogen storage. In the framework of the semi-empirical TBMD method, the methane dissociation reaction occurring at the SWCNTs wall have been investigated. By combining canonical molecular dynamic simulations and damped dynamics it has been demonstrated that the dissociation proceeds with small changes of the bonding energy if it is assumed that the methane molecule escapes from the physisorption equilibrium state through the relevant energy barrier towards the nanotube wall. The dissociation reaction transition states have been thoroughly investigated in terms of the CNTs electronic structure properties and their relationship with the observed bond breaking and forming events. On the other hand the possibility of employing an alkali metal decorated SWCNT as a methane storage media have been

investigated through DFT calculations, Ca decorated SWCNT, in fact, can be successfully employed for CH_4 storage purposes, as they evidence an improved methane uptake (up to six molecules) per Ca impurity. Similarly to the molecular hydrogen adsorption case, the electronic empty *d* states of Ca are mostly responsible of the enhanced adsorption via a Kubas-type interaction involving the methane molecular orbitals and the *s*, *p* and *d* states of Ca.

Functionalization of semiconducting surfaces with self-assembled-monolayers (SAMs) for nano-fluidic and FET applications.

There is a great interest for the physics of the solid-liquid interfaces, mainly due to the recent developments in nano-technology that have made possible the fabrication of devices integrating deterministic networks of nano- channels. This new class of devices has a potential role in the sieving mechanisms of bio- molecules and in the nano-fluidic at the nano-scale. Quantum mechanical investigations of Si(111), chemically processed with Self-Assembled Monolayers (SAMs) of long chains of alkaloid molecule have been carried out, focussing the interest in the growth process of such auto-assembled polymer surfaces on a substrate, which deeply affects their chemical and physical properties (chemical reactivity or wetting) and the influence of defect rich structures on the solid-liquid slipping. Octadecyltrichlorosilane (OTS) coatings on a Si surface at different coverage ratios have also been considered; the possibility of multiple covalent bonding between a (111) Si surface and a OTS molecule has been explored using first principles calculations based on the DFT, as a possible source of irregularities and disorder. All the structures studied exhibit negative adsorption energy, indicating that they are stable and may form easily during deposition. The DFT charge density has been used to calculate the partial dipole being finalized to predict reliable values of the work function change with respect to the hydrogenated Si surface. This quantity has been related to the surface electrostatic dipole through a linear relationship that has been established by studying various partial coverage values and adsorption configurations. For all the adsorption configurations examined, the measured electron work function of the coated surface is lowered with respect to the hydrogenated surface, thus increasing the hole isolation behaviour. A simple superposition toy model has been tested on the various configurations considered, showing that it is appropriate to predict the surface dipole and, through the linear relationship, the work function; then this model has been used to extrapolate the surface dipole and the work function to full coverage, giving $\Delta\Phi$ for uniform coatings and showing that eventual poor self-assembling features or incomplete domain boundaries may severely affect the device performances.

Specific surface recognition by hydratated amino-acids.

In last years the simultaneous enhancement of both technological experimental instrument and the computational resources to investigate the nano-scale world, allowed the scientists to lead new kind of applications depending on the particular interactions between organic/inorganic compounds. In particular there is a new wide area of investigation regarding the functionalization of metalic/oxide surfaces with biological matter, in order to develop new kind of sensor and generally nano-devices able to implement or supply part of currently science fields. The specific aim of the work done in such scientific area is a DFT study the interaction between several selected charged amino acids of technological interest (i.e. lysine, aspartate and arginine) and a hydrated TiO_2 anatase surface. Such work is a part of a wider project aimed to understand and investigate material surfaces behaviour interacting with biological matter: the META (Material Enhancement for Technological Applications) Project, carried in collabortion with the NAST Center (ENEA and University of Tor Vergata), and it is focussed on utilizing the inherent self-assembling properties of biological molecole to build functional nano-devices. The numerical simulations have given a first interpretation of the selective interaction between the charged amino acids and the anatase surface; being these amino acids the potential responsible of the interactions between physiological peptides and inorganic materials. In all the cases studied, the amino acids strongly interact with the surface; however either the aspartate molecule or the lysine molecule show a lower adsorption energy on the hydrated surface with respect to the dry one, while in the arginine case the opposite occurs. This fact is probably due to the different adsoprtion interactions with the hydrated surface, experienced by aspartate and lysine with respect to arginine. In the latter case water enforces the adsorption energy, resulting in a higher stability. The results obtained have been recently submitted for publication.

LIST OF PUBLICATIONS

- Authors: F. Gala and G. Zollo
- Title: Augmented methane adsorption at Ca decorated carbon nanotubes—a DFT study
- Journal: Journal of Physics D: Applied Physics **47**, 075305
- Year: 2014

- Authors: G. Zollo and F. Gala
- Title: Atomistic of gas adsorption in carbon nano-structures
- Book: Carbon nanomaterials for gas adsorption, edited by Maria Letizia Terranova, Silvia Orlanucci

	and Marco Rossi, Pan Stanford Publishing
• Year	2012
• Authors	F. Gala and G. Zollo
• Title	Work Function Dependence on the Adhesion Configuration of Self- Assembled Alkyl-Silane Coatings of (111) Silicon Surface
• Journal	Journal of Physical Chemistry C **116**, 24935
• Year	2012
• Authors	G. Zollo and F. Gala
• Title	Atomistic modeling of gas adsorption in nanocarbons
• Journal	Journal of Nanomaterials **2012**, 152489
• Year	2012
• Authors	L. Bagolini, F.Gala and G. Zollo
• Title	Methane cracking on single-walled carbon nanotubes studied by sempi-empirical tight binding simulations
• Journal	Carbon **50**, 411
• Year	2012
• Authors	G. Zollo and F. Gala
• Title	Migration barriers of neutral As di-interstitials in GaAs
• Journal	New Journal of Physics **14**, 053036
• Year	2012
• Authors	G. Zollo and F. Gala
• Title	Calculation of di-interstitial diffusion barriers in GaAs by density functional theory
• Book	ENEA-High performance computing on CRESCO infrastructure: research activities and results 2010-2011
• Year	2012
• Authors	F. Gala and G. Zollo
• Title	Hydrophobic coatings on hydrogenated (111) silico surface
• Book	ENEA-High performance computing on CRESCO infrastructure: research activities and results 2010-2011
• Year	2012
• Authors	F. Gala and G. Zollo
• Title	Functionalization of hydrogenated (111) silicon surface with hydrophobic polymer chains
• Journal	Physical Review B **84**, 195323
• Year	2011
• Authors	M.Chinappi, F.Gala, G. Zollo and C.M. Casciola
• Title	Tilting angle and water slippage over hydrophobic coatings
• Journal	Philosophical Transactions of the Royal Society of London Series A **369**, 2537
• Year	2011
• Authors	F. Gala and G. Zollo
• Title	Nucleation and first-stage growth processes of extrinsic defects in GaAs triggered by self-interstitials
• Journal	Physical Review B **80**, 174113
• Year	2009
• Authors	G. Zollo and F. Gala
• Title	Properties of charged intrinsic di-interstials in GaAs
• Journal	Physical Review B **77**, 094125
• Year	2008

• Authors	G. Zollo and F. Gala
• Title	Stability of I_3 complexes in III-V compound semiconductors by tight-binding molucular dynamics
• Journal	Physical Review B **75**, 115205
• Year	2007

• Authors	G. Zollo and F. Gala
• Title	Stability of I_3 complexes in III-V compound semiconductors by tight-binding molucular dynamics
• Journal	Physical Review B **75**, 115205
• Year	2007

ROMA 02/04/2014
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