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Giuseppe Fisicaro

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Zona Industriale Strada VIII, 5, 95121, Catania, Italy

WORK EXPERIENCE

28/11/2019 – CURRENT – Catania, Italy

RESEARCHER – CNR INSTITUTE FOR MICROELECTRONICS AND MICROSYSTEMS (CNR-IMM)

My research interests concern the theoretical study as well as the development of models and codes to investigate materials design and discovery, materials properties and process simulations for clean energy and micro/nanoelectronic applications. I focus my research on materials and processes at various scales, that are from the atomistic level with ab-initio calculations or artificial intelligence machine learning techniques to the meso-scale with Monte Carlo, continuum modelling or multi-scale techniques for process simulations. Investigation of material properties and processes with *ab-initio* structure predictions and first-principle electronic-structure methodologies (DFT, DFTB+ and MD). Ab-initio DFT and structure predictions code developments. Systems of interest: perovskite materials for solar cell applications, TiO_2 surfaces and clusters for water splitting and electrocatalysis, silicon carbide for power electronics, hydrogen storage and production for hydrogen economy, nucleation thermodynamics and kinetics of clusters, solid/liquid interfaces.

https://hq.imm.cnr.it | Z.I. VIII strada, 5, 95121, Catania, Italy

05/09/2018 – 27/11/2019

POST-DOC RESEARCHER – CNR INSTITUTE FOR MICROELECTRONICS AND MICROSYSTEMS (CNR-IMM)

Research activity within the European Project H2020 “CHALLENGE” - 3C-SiC Hetero-epitaxiALLy grown on silicon compliancE substrates and 3C- SiC substrates for sustaiNable wide-band-Gap powEr devices. Multiscale modeling, ab-initio density functional theory calculations together with kinetic Monte Carlo simulations for silicon-carbide materials and nanosystems.
Ab-initio structure predictions and first-principle electronic-structure methodologies (DFT, DFTB+ and MD) to investigate various systems of interest in material science. Investigation of perovskite materials for solar cell applications. TiO2 surfaces and clusters for water splitting. Development of implicit solvation models for ab-initio calculations. Full extension of the BigDFT suite to non-orthorhombic cells.

https://hq.imm.cnr.it | Z.I. VIII strada, 5, 95121, Catania, Italy

17/03/2014 – 31/08/2018

POST-DOC RESEARCHER – DEPARTMENT OF PHYSICS - UNIVERSITY OF BASEL

Post-doc researcher within the Swiss PASC project "ENVIRON: A Library for Complex Electrostatic Environments in Electronic-structure Simulations" at the Department of Physics, University of Basel within the Prof. Dr. Stefan Goedecker's group. The project was in collaboration with Prof. Dr. Nicola Marzari Theory and Simulation of Materials Institute of Materials EPFL, Lausanne and Prof. Dr. Juerg Hutter Physics Department University of Zurich.
We developed *from scratch* an electrochemical library which extends first-principle electronic-structure codes to complex-wet environments. The library is able to solve both the generalized Poisson and the Poisson-Boltzmann equations, allowing to handle both neutral and ionic solutions implicitly in DFT calculations. We developed, parametrized and tested an implicit solvation model named ``soft-sphere''. *Ab -initio* structure predictions and first-principle electronic-structure methodologies (DFT, DFTB+ and MD) to investigate various systems of interest in material science. Full extension of the BigDFT suite to non-

orthorhombic cells. Teaching assistant for several courses of computational physics and electronic-structure calculations.

https://comphys.unibas.ch/ | Klingelbergstrasse 82, 4056, Basel, Switzerland

13/10/2012 – 28/02/2014

POST-DOC RESEARCHER – CNR INSTITUTE FOR MICROELECTRONICS AND MICROSYSTEMS (CNR-IMM)

Awarded of a research grant N° BS. IMM006/2012/CT, Prot. N° 0003890 23/07/2012 published on Italian G.U. N° 60 the 03/08/2012 "Formazione di esperti per la Progettazione, Realizzazione e Caratterizzazione di celle solari e sistemi concentratori" (PON01_01725).
Simulation of dopant-defect evolution under thermal laser annealing processes both in solid and liquid phase.
Simulation of the feature profile evolution in plasma etch-dep processes. Development of kMC codes and physical models based on surface phenomena (neutral absoption, detachment, ion enhanced stitching and detachment, etc). Partecipation in projects: ENIAC Program Implementing Manufacturing science solutions to increase equiPment pROductiVity and fab pErformance (IMPROVE).
Study of light trapping and absorption in multylayer solar cells for photovoltaic applications by means of codes developped in matlab enviroment.
Development and implementation of a simulation method overcoming the limits of fluid-flow based approaches for dielectrophoretic device investigations. Development of a three dimensional Monte-Carlo-Poisson simulator for a colloidal system at a particle resolution. Investigation of circulation tumor cell trapping induced by dielectrophoretic forces in real devices by means of continuum models. Use of the Comsol platform.

https://hq.imm.cnr.it | Z.I. VIII strada, 5, 95121, Catania, Italy

15/01/2012 – 12/10/2012

POST-DOC RESEARCHER – CNR INSTITUTE FOR MICROELECTRONICS AND MICROSYSTEMS (CNR-IMM)

Awarded of a research grant N° BS IMM005/2011/CT prot. n. 0000106 12-01-2012 inside the European research project "Advanced Technology Modeling for Extra-Functionality Devices – Enlarged EU ATEMOX Grant Agrement N° 287669".
Investigation of system kinetics in extremely out-of-equilibrium conditions induced by laser irradiation by means of kinetic Monte Carlo simulations and continuum modeling. Study of defects evolution and dopant activation in silicon implanted substrates during thermal laser annealing processes. Study of stress effects induced by laser irradiation. Development *from scratch* of kMC codes as well as continuum models. Planning and coordination of experiments as well as drawing up of technical reports and regular publications. Partecipation in projects: European Seventh Framework Programme (FP7/2007-2013) under the grant agreement n. 258547 ATEMOX (Advanced Technology Modeling for Extra-Functionality Devices), in collaboration with several european parteners.

https://hq.imm.cnr.it | Z.I. VIII strada, 5, 95121, Catania, Italy

01/02/2011 – 31/05/2011

VISITING PHD STUDENT – DEPARTMENT OF ELECTRONICS, UNIVERSITY OF VALLADOLID

Four months spent as visiting PhD student at the department of electronics at the University of Valladolid (Spain) under the supervision of Prof. Lourdes Pelaz. The collaboration has been focused on the theoretical characterization of dopant-defect system in implanted silicon under an ultra-fast heating process, i.e. laser irradiation. Development, implementation and calibration of a Partial Differential Equation model of dopant activation in silicon under laser treatment. Use of the SRIM code based on the Binary Collision Approximation. Implementation and calibration *from scratch* of a kinetic Monte Carlo code fot dopant-defects in silicon under laser annealing.

Valladolid, Spain

01/01/2008 – 28/02/2014

WIND ORCHESTRA CONDUCTOR – ASSOCIAZIONE MUSICALE "V. BELLINI"

I covered the position of conductor and music director of the wind orchestra "V. Bellini" of Buccheri (Sr, Italy). In the same period I worked as a teacher of trombone and brass instruments in the same institution.

Buccheri (Sr), Italy

EDUCATION AND TRAINING

10/05/2019 – CURRENT

ABILITAZIONE SCIENTIFICA NAZIONALE

Abilitazione Scientifica Nazionale - SETTORE CONCORSUALE 02/B2 FISICA TEORICA DELLA MATERIA. Valida dal 10/05/2019 al 10/05/2025 (art. 16, comma 1, Legge 240/10) per le funzioni di Professore Universitario di seconda fascia.

01/11/2008 – 31/10/2011 – Catania, Italy

DOCTOR OF PHILOSOPHY IN PHYSICS – University of Catania - Department of Physics and Astronomy

Viva voce defence on 01/02/2012.
Thesis on "Micro-structural modifications of semiconductor systems under irradiation: experiment, modeling and simulation analysis". Advisors Prof. G Piccitto (Department of Physics, University of Catania) and Dr. A. La Magna (CNR-IMM Catania).
Research on the micro-structural modifications of semiconductor systems during Laser Thermal Annealing processes. Post-implant kinetics of the defect-dopant system in the extremely far from the equilibrium conditions caused by laser irradiation both in the non-melting and melting regime. Accurate study of the feasibility of laser irradiation as a heat source for real patterned substrates for the case of SiGe and Ge based MOS devices. Developping of a continuum simulation code which simulates the interaction between the laser light and the transistor periodic structure in order to estimate the heat source as well as the heat diffusion, phase changes and material redistribution under irradiation.

01/01/2013 – 18/12/2013 – Catania, Italy

QUALIFICATION FOR TEACHING IN SECONDARY SCHOOLS - MATHEMATICS AND PHYSICS – University of Catania

Qualification for teaching in secondary schools Mathematics and Physics obtained after passing a public selection and an one year university course (Tirocinio Formativo Attivo - TFA).

01/10/2000 – 14/07/2008 – Catania, Italy

MASTER'S DEGREE IN PHYSICS – Department of Physics and Astronomy - University of Catania

Master's Degree in Physics - Top grade - Specialization in physics of condesed matter, semiconductor physics, theoretical and computational physics. Thesis "Evolution of defect-impurity systems in silicon under laser irradiation" supervisors Prof. G Piccitto (Department of Physics, University of Catania) and Dr. A. La Magna (CNR-IMM Catania).

01/10/1994 – 01/10/2000 – Catania, Italy

MASTER'S DEGREE IN MUSIC - TROMBONE – Istituto Musicale Pareggiato “V. Bellini”

LANGUAGE SKILLS

Mother tongue(s): **ITALIAN**

Other language(s):

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken production	Spoken interaction	
ENGLISH	B2	B2	B2	C1	B2
GERMAN	A2	A2	A2	A2	A2

Levels: A1 and A2: Basic user; B1 and B2: Independent user; C1 and C2: Proficient user

DIGITAL SKILLS

Microsoft Office | Microsoft Word | Microsoft Excel | Microsoft Powerpoint | Outlook | programming (Python, Fortran, Matlab)

PROJECTS

Projects

Supporting research tasks of the European Project H2020 “CHALLENGE” - 3C-SiC Hetero-epitaxiALLy grown on silicon compliancE substrates and 3C- SiC substrates for sustaiNable wide-band-Gap powEr devices GRANT AGREEMENT N. 720827 – CUP: B66J16001480006. Ab-initio density functional theory calculations together with Monte Carlo simulations for silicon-carbide materials and nanosystems.

Projects

Swiss PASC project "ENVIRON:A Library for Complex Electrostatic Environments in Electronic-structure Simulations".
The computational study of chemical reactions in complex, wet environments is critical for applications in many fields, and of cross-disciplinary interest to physics, chemistry, materials science, chemical engineering, and biology. Driven by very recent advances and developments in this field, we propose to develop and distribute an open-source library of verified and validated electrochemical andsolvation modules, able to run efficiently on advanced computing architectures, and interface it with some of the core electronic-structure codes developed or co-developed in Switzerland - namely ABINIT, BigDFT, CP2K, and Quantum ESPRESSO. Given its documented and open-source nature, it is also expected that such tool will become of wide use outside these communities, and be adopted by other public or distributed codes. The core objective of this library will be to describe complex electrostatic environmentswhere an explicit solvent becomes implicit, with a position-dependent dielectric constant, or where mobile ions can shield the charge or multipoles of the system of interest; it will embed the quantum simulation engines into a robust and efficient Poisson-Boltzmann solver that has been extensively verified and validated.

Projects

Swiss NCCR MARVEL project (http://nccr-marvel.ch). Centre on Computational Design and Discovery of Novel Materials, that has been cre- ated by the Swiss National Science Foundation in May 2014. The goal of the NCCR MARVEL is to radically transform and accelerate invention and discovery in science and technology, and espe- cially to transform and accelerate the design and discovery of novel materials in order to achieve improved properties and performance, or to witness the emergence of original physical proper- ties. We will achieve this goal by exploiting the predictive accuracy that quantum-mechanical simulations have now reached for realistic, complex systems, the treasure trove of ever-increasing computational power ideally suited to intrinsically parallel problems, and the powerful synergies arising with the computer science of heterogeneous data management, data mining, and machine learning. EPFL acts as the leading house, and it is directed by Nicola Marzari, but it involves 41 principal investigators across 12 Swiss Institutions: the two Federal Institutes of Technology in Lausanne and Zurich (EPFL and ETHZ), six universities in Basel, Bern, Fribourg, Geneva, Svizzera Italiana, and Zurich (UNIBAS, UNIBE, UNIFR, UNIGE, USI, UZH), the Swiss Na- tional Supercomputing Centre (CSCS), the research laboratories of IBM Zurich, the two federal research institutes, the Paul Scherrer Institute (PSI), and the Swiss Federal Laboratories for Materials Science and Technology (Empa). The applicant integrated his research in Basel to the various work-packages of the Marvel project.

Projects

The study of defects evolution and dopant activation in silicon implanted substrates during thermal laser annealing processes by means of kinetic Monte Carlo simulations and continuum modeling as well as the study of stress effect induced by laser irradiation were carried out inside the European Seventh Framework Programme (FP7/2007-2013) under the grant agreement n. 258547 ATEMOX (Advanced Technology Modeling for Extra-Functionality Devices), in collaboration with several european parteners. FRENDTECH and ATOMICS with major contributions by the current partners, process simulation has been brought to a state which allows in industrial environments a sufficiently accurate simulation of doping profiles in advanced CMOS technologies. Important electrical characteristics of core CMOS devices can now be predicted from scratch or with a minimum calibration effort. However, concepts towards low-power electronics, smart power applications, CMOS image sensors, and CMOS derivatives providing extra functionalities are still not sufficiently supported by TCAD. This concerns especially the prediction of leakage currents in such or parasitic devices caused by electrically active defects that remain after processing, and alternative doping techniques like plasma immersion ion implantation, low-temperature implantation, diversified cocktail implants and laser annealing which are considered for low-leakage ultra shallow junctions. The lack of suitable models that can be used in the early stages of industrial R&D inhibits the necessary cost reduction in the development of devices for which Europe is still at the forefront. Funded within the ICT theme of the Seventh Framework Programme of the EC, the ATEMOX project develop the full set of missing models and implement and include them into the Sentaurus TCAD platform of Synopsys so that they are of immediate value to the European semiconductor industry. The integrated models has been finally evaluated by STMicroelectronics with respect to industrial needs. To reach these ambitious goals, a consortium of European companies active in complementary fields of competence (STMicroelectronics: device manufacturing, Synopsys: TCAD software, Exico, IBS: equipment production, Probion, Semilab: characterization) and leading European research institutes (CNRS-LAAS/CEMES, CNR-IMM, ETH-Zurich, Fraunhofer-IISB, Univ. Newcastle) has been formed which, together, is well prepared to expertly cover all fields from experiment via characterization and modelling to simulation.
http://www.atemox.eu/

ORGANISATIONAL SKILLS

Organisational skills

Leadership, good organisational and team-leading skills gained as president, music director and orchestra conductor of the wind orchestra "V. Bellini" of Buccheri, Siracusa (Italy) responsible for a team of 35 people from January 2004 to present.

COMMUNICATION AND INTERPERSONAL SKILLS

Communication and interpersonal skills

Good communication skills gained through my experience as post-doc researcher.
Excellent contact skills gained through my experience as post-doc researcher as well as music teacher and orchesta conductor.

JOB-RELATED SKILLS

Job-related skills

Considering the peculiarity of my research field which concerns theoretical investigation of Condensed Matter Physics by means of simulations and modelling, my principal attitude and skills focus on writing and developping *from scratch* codes and models, in particular the programming work is my favorite.
Moreover, my skills concern teaching or explaining in detail to individuals and group, sharing or communicating well in speech and writing with individuals and group, helping people network or make contact with each other, leading or directing or chairing a discussion with groups, mediate between parties help solve disputes with groups, producing, creating, formulating or devising original ideas or concepts.
Drawing up scientific and technical reports or regular publications in english. I am author of forty publications published in several internationl journals (JCR). Among them Applied Physics Reviews, Nano Letters, Physical Review Letters, Physical Review Materials, Scientific Report, Journal of Chemical Theory and Computation, Journal of Chemical Physics, Physical Review E, Applied Physics Letters, Applied Physics Express, Journal of Applied Physics, etc. I presented in the past years my work as oral presentations in several international conferences (APS March Meeting, Psi-k Conference, CECAM workshop, E-MRS Spring Meeting, SISPAD, LMP Conference, IIT held in France, Spain, Japan and United States).

PERSONAL DATA

Data consent

According to law 679/2016 of the Regulation of the European Parliament of 27th April 2016, I hereby express my consent to process and use my data provided in this CV.

Scientific curriculum

Giuseppe Fisicaro

Contents

1 Narrative curriculum

The scientific curriculum of Giuseppe Fisicaro is documented by the list of publications on international journals, all submitted to review processes. The applicant published more than 50 papers, attended 40 conferences and held 5 seminars at different institutions.

Giuseppe Fisicaro got his **master's degree in physics**, top grade, at the University of Catania Department of Physics (Italy) with a specialization in physics of condesed matter, semiconductor physics, theoretical and computational physics the 14th July 2008. The master thesis was entitled "Evolution of defect-impurity systems in silicon under laser irradiation", with the supervisor of Prof. G Piccitto (Department of Physics, University of Catania) and Dr. A. La Magna (CNR-IMM Catania).

Subsequently he got the **Philosophiae Doctor degree (PhD) in physics** cum laude the first of February 2012 (viva voce defense) at the Department of Physics, University of Catania. His PhD has been carried out in collaboration with the National Research Council (Italian: Consiglio Nazionale delle Ricerche, CNR) Institute for Microelectronics and Microsystems (CNR-IMM) of Catania. The title of the thesis was "Micro-structural modifications of semiconductor systems under irradiation: experiment, modeling and simulation analysis", developed under the supervision of Prof. Dr. G Piccitto and Dr. A. La Magna. During his PhD period the applicant has strengthened his program- ming skills as well as experiment-simulation interfacing research work. He developed an atomistic kinetic Monte Carlo code for dopant-defects evolution during laser thermal annealing and a cou- pled Monte Carlo-Poisson method for the simulation of particle-particle effects in dielectrophoretic devices. These atomistic investigations have been extensively integrated with continuum mean field approaches, developing continuum reaction-diffusion models for the dopant-defects annealing process both in solid and liquid phase. The computational study has been coupled with target experiments, and the applicant participated in the planning of the whole experimental activity.

After his PhD, he has been awarded of two research grants (**post-doc**) at the CNR-IMM in the field of process simulations of dopant-defects under laser annealing, plasma etching-deposition processes, light trapping and absorption in multilayer solar cells and Monte Carlo-Poisson simulator for colloidal systems, exploiting its atomistic and continuum modeling background.

In March 2014 he joined the Prof. Dr. Stefan Goedecker's group in Basel (Switzerland) as **post-doc researcher**. He developed from scratch an electrochemical library which extends first-principle electronic-structure codes to complex-wet environments. The library is able to solve both the generalized Poisson and the Poisson-Boltzmann equations, allowing to handle implicitly both neutral and ionic solutions in density functional theory (DFT) calculations. He developed, parameterized and tested an implicit solvation model named "soft-sphere". This model is implemented in state-of-the-art first principle DFT codes like BigDFT, Quantum Espresso, ONETEP, and so on. In Basel he complemented his theoretical and computational skills with first-principle electronic-structure methodologies and structure predictions at various level of theory. He has been assistant for several courses, like computational physics and electronic-structure calculations.

He has been awarded as principal investigator for the computational project "Effects of complex liquid environments on material properties", a **computational project for node/hours** at the Swiss National Supercomputing Center (CSCS) in Switzerland under Project ID s869. He got 0.8 million node hours (9.6 million cpu hours) on Daint HPC machine, from 1 October 2018 to 30 September 2020.

After the Basel experience, he has been awarded of one research grants (**post-doc**) at the CNR-IMM of Catania, supporting research tasks of the European Project H2020 CHALLENGE. Here he performed ab-initio density functional theory calculations together with Monte Carlo simulations to silicon-carbide materials and nanosystems.

Starting from 28 November 2019 he is **permanent researcher** at the CNR, performing his studies at the Institute for Microelectronics and Microsystems of Catania.

His research interests lie on the theoretical study as well as the development of models and codes to investigate materials design and discovery, materials properties and process simulations for clean energy and micro/nanoelectronic applications. He focus his research on materials and processes at various scales, that are from the atomistic level with ab-initio calculations or artificial intelligence machine learning techniques to the meso-scale with Monte Carlo, continuum modelling or multi-scale techniques for process simulations. Among various projects, he pursues the investigation of material properties and processes with ab-initio structure predictions and first-principle electronic-structure methodologies. He is involved in the development of various codes and models for ab-initio DFT calculations and structure predictions (BigDFT software package) and Monte Carlo kinetics simulations (MulSKIPS code). Systems of interest: perovskite materials for solar cell applications, TiO_2 surfaces and clusters for water splitting and electrocatalysis, silicon carbide for power electronics, hydrogen storage and production for hydrogen economy, nucleation thermodynamics and kinetics of clusters, solid/liquid interfaces.

2 Projects for computational hours

- Principal Investigator for the computational project "Effects of complex liquid environments on material properties", a computational project for node/hours at the Swiss National Supercomputing Center (CSCS) in Switzerland under Project ID s869. Computational hours 0.8 million node hours (9.6 million cpu hours) on Daint HPC machine from 1 October 2018 to 30 September 2020. Projects: Many important physicochemical processes take place in solution, both in the context of basic as well as industrial research. Here we aim at developing and assessing a groundbreaking theoretical/computational paradigm to study complex wet environment effects on material properties at an atomistic level. Since material properties are ultimately related to the underlying atomic structure, we plan to extend current ab-initio structure prediction codes to wet environments. Solvents will be described by a recently developed implicit solvation model, called "soft-sphere". The approach aims at overcoming all drawbacks that hinder the application of structure predictions to wet environments. Among them, the explosion of the system size when explicit solvent molecules are considered, which makes simulations extremely costly from a computational point of view. A first application of the proposed computational paradigm has been demonstrated successful at describing surface reconstructions of fluorite in water. The methodology will be benchmarked with target experiments and molecular dynamics simulations. Molecular doping of silicon, small TiO_2 clusters, and surfaces in various solvents

will be some of the systems to be investigated. Target experiments carried out by the applicant partner CNR-IMM in Catania, Italy.

3 Post-doc career

- Post-doc researcher at CNR Institute for Microelectronics and Microsystems from 5 September 2018 to 27 November 2019.
- Post-doc researcher within the Swiss PASC and MARVEL projects at the Department of Physics, University of Basel (Switzerland) within the Prof. Dr. Stefan Goedecker's group from 17 March 2014 to 31 August 2018.
- Post-doc researcher at CNR Institute for Microelectronics and Microsystems from 17 February 2014 to 16 Marzo 2014.
- Awarded of a research grant (Post-doc) N° BS. IMM006/2012/CT, Prot. N° 0003890 23/07/2012 published on Italian G.U. N° 60 the 03/08/2012 "Formazione di esperti per la Progettazione, Realizzazione e Caratterizzazione di celle solari e sistemi concentratori" (PON01-01725) at the CNR Institute of Microelectronic and Microelectric systems, Catania 13 October 2012 to 31 December 2013.
- Awarded of a research grant (Post-doc) N° BS IMM005/2011/CT prot. n. 0000106 12-01-2012 inside the European research project "Advanced Technology Modeling for Extra-Functionality Devices – Enlarged EU ATEMOX Grant Agrement N° 287669" at the CNR Institute of Microelectronic and Microelectric systems, Catania from 15-01-2012 to 12 October 2012.

4 Publications on International Peer Review Journals

- F. La Via, M. Zimbone, C. Bongiorno, A. La Magna, G. Fisicaro, I. Deretzis, V. Scuderi, C. Calabretta, F. Giannazzo, M. Zielinski, R. Anzalone, M. Mauceri, D. Crippa, E. Scalise, A. Marzegalli, A. Sarikov, L. Miglio, V. Jokubavicius, M. Syväjärvi, R. Yakimova, P. Schuh, M. Schöler, M., Kollmuss, P. Wellmann "New approaches and understandings in the growth of cubic silicon carbide" Materials, **14**(18), 5348 (2021).
- S. Sanzaro, C. Bongiorno, P. Badalà, A. Bassi, I. Deretzis, M. Enachescu, G. Franco, G. Fisicaro, P. Vasquez, A. Alberti, A. La Magna "Simulations of the ultra-fast kinetics in Ni-Si-C ternary systems under laser irradiation" Materials, **14**(16), 4769 (2021).
- I. Deretzis, C. Bongiorno, G. Mannino, E. Smecca, S. Sanzaro, S. Valastro, G. Fisicaro, A. La Magna, A. Alberti "Exploring the structural competition between the black and the yellow phase of $CsPbI_3$" Nanomaterials, **11**(5), 1282 (2021).
- G. Mannino, I. Deretzis, E. Smecca, F. Giannazzo, S. Valastro, G. Fisicaro, A. La Magna, D. Ceratti, A. Alberti "$CsPbBr_3$, $MAPbBr_3$, and $FAPbBr_3$ bromide perovskite single crystals: Interband critical points under dry N_2 and optical degradation under humid air" Journal of Physical Chemistry C, **125**(9), 4938-4945 (2021).
- A. Alberti, E. Smecca, I. Deretzis, G. Mannino, C. Bongiorno, S. Valastro, S. Sanzaro, G. Fisicaro, A.K. Jena, Y. Numata, Z. Guo, C. Spinella, T. Miyasaka, A. La Magna "Formation of $CsPbI_3$ γ-Phase at 80 °C by Europium-Assisted Snowplow Effect" Advanced Energy and Sustainability Research **2**, 2100091 (2021).
- L. Marqués, M. Aboy, P. López, I. Santos, L. Pelaz, G. Fisicaro "Atomistic modeling of laser-related phenomena" Laser Annealing Processes in Semiconductor Technology, Book Chapter 3, Woodhead Publishing, 79-136 (2021).
- S. Filice, R. Fiorenza, R. Reitano, S. Scalese, S. Sciré, G. Fisicaro, I. Deretzis, A. La Magna, C. Bongiorno, G. Compagnini "TiO_2 Colloids Laser-Treated in Ethanol for Photocatalytic H_2 Production" ACS Applied Nano Materials, **3**(9), 9127-9140 (2020).

- A. Sciuto, I. Deretzis, G. Fisicaro, S.F. Lombardo, A. La Magna, M.G. Grimaldi, K. Huet, B. Lespinasse, A. Verstraete, B.Curvers, I. Bejenari, A. Burenkov, P. Pichler "Advanced simulations on laser annealing: Explosive crystallization and phonon transport corrections" International Conference on Simulation of Semiconductor Processes and Devices, SISPAD, 2020-September, 71-74 (2020).
- G. Fisicaro, C. Bongiorno, I. Deretzis, F. Giannazzo, F. La Via, F. Roccaforte, M. Zielinski, M. Zimbone, A. La Magna "Genesis and evolution of extended defects: The role of evolving interface instabilities in cubic SiC" Applied Physics Reviews, **7**(2), 021402 (2020) **Featured Article**.
- L.E. Ratcliff, W. Dawson, G. Fisicaro, D. Caliste, S. Mohr, A. Degomme, B. Videau, V. Cristiglio, M. Stella, M. D'Alessandro, S. Goedecker, T. Nakajima, T. Deutsch, L. Genovese "Flexibilities of wavelets as a computational basis set for large-scale electronic structure calculations" Journal of Chemical Physics, **152**(19), 194110 (2020).
- M. Zimbone, E.G. Barbagiovanni, C. Bongiorno, C. Calabretta, L. Calcagno, G. Fisicaro, A. La Magna, F. La Via "Generation and Termination of Stacking Faults by Inverted Domain Boundaries in 3C-SiC" Crystal Growth and Design, **20**(5), 3104-3111 (2020).
- A. Sciuto, I. Deretzis, G. Fisicaro, S.F. Lombardo, M.G. Grimaldi, K. Huet, B. Curvers, B. Lespinasse, A. Verstraete, A. La Magna "Phononic transport and simulations of annealing processes in nanometric complex structures" Physical Review Materials, **4**(5), 056007 (2020).
- G. Fisicaro, A. La Magna, A. Alberti, E. Smecca, G. Mannino, I. Deretzis "Local Order and Rotational Dynamics in Mixed A-Cation Lead Iodide Perovskites" Journal of Physical Chemistry Letters, **11**(3), 1068-1074 (2020).
- G. Fisicaro, S. Filice, S. Scalese, G. Compagnini, R. Reitano, L. Genovese, S. Goedecker, I. Deretzis, A. La Magna "Wet Environment Effects for Ethanol and Water Adsorption on Anatase TiO_2 (101) Surfaces" Journal of Physical Chemistry C, **124**(4), 2406-2419 (2020).
- R.A. Puglisi, S. Caccamo, C. Bongiorno, G. Fisicaro, L. Genovese, S. Goedecker, G. Mannino, A. La Magna "Direct observation of single organic molecules grafted on the surface of a silicon nanowire" Scientific reports **9**(1), 5647 (2019).
- M. Zimbone, M. Zielinski, C. Bongiorno, C. Calabretta, R. Anzalone, S. Scalese, G. Fisicaro, A. La Magna, F. Mancarella, F. La Via "3C-SiC growth on inverted silicon pyramids patterned substrate" Materials, **12** (20) (2019).
- S.F. Lombardo, G. Fisicaro, I. Deretzis, A. La Magna, B. Curver, B. Lespinasse, K. Huet "Theoretical study of the laser annealing process in FinFET structures" Appl. Surf. Sci. **467**, 666-672 (2019).
- O. Andreussi, N.G. Hormann, F. Nattino, G. Fisicaro, S. Goedecker, N. Marzari "Solvent-aware interfaces in continuum solvation" J. Chem. Theory Comput. **15**(3), 1996-2009 (2019).
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PhD Thesis: G. Fisicaro "Micro-structural modifications of semiconductor systems under irradiation: experiment, modeling and simulation analysis". Philosophiae Doctor degree in Physics cum laude at the Department of Physics, University of Catania. Viva voce defense 01-02-2012.

5 Awards

- "Seal of Excellence" from the European Commission - Research and Innovation - for the project proposal 799206, COMPWET "Complex wet environments effects on material properties at atomistic level" submitted under the Horizon 2020's Marie Skłodowska-Curie actions call H2020-MSCA-IF-2017 of 14 September 2017. The Seal of Excellence is the high-quality label awarded to projects submitted to Horizon 2020 which were deemed to deserve funding but did not receive it due to budget limits (scored 85% or above). The Seal of Excellence is recognition that your project proposal was evaluated as excellent in a highly competitive evaluation process and is recommended for funding by other sources, since Horizon 2020 resources available for this specific call were already allocated following a competitive ranking. The certificate can be used to increase the visibility and reputation of the project proposal and possibly attract the interest of public or private investors.

- Best poster presentation "Soft-sphere continuum solvation in electronic structure calculations" on "Four Marvel Retreat" 07/09/2017, Lausanne, Switzerland.
- Eligible but non-winner (ranked seventh after all exams, 3rd August 2017) for the profile of permanent researcher - III professional level Notice of application 367.10 DSFTM IMM RIC, at the Institute for Microelectronics and Microsystems - Catania, member of the Department of Physical Sciences and Technologies of the matter of the National Research Council, whose notice was published in the Official Gazette of the Italian Republic - IV Special Series n. 24 on 25/03/2016.

6 Invited presentations

- "CECAM workshop: Liquid/solid interfaces from spectroscopy to simulations" 25-27/01/2016, Lausanne, Switzerland. Invited oral presentation: G. Fisicaro et al. "Complex wet-environments in electronic-structure calculations" (https://www.cecam.org/workshop-1-1168.html?aid=25039).
- "Structure predictions and electronic-structure calculations in complex wet environments", CNR-IMM Catania, Italy (04/08/2017).
- "A Generalized Poisson and Poisson-Boltzmann solver in wet-environments electronic-structure calculations", CEA Grenoble, France (September 2015).
- "Continuous modeling of dopant activation on laser irradiated silicon", Department of Electronic University of Valladolid (March 2011).
- "Kinetic of dopant-defect systems under laser irradiation", CNR-IMM Catania (December 2010).
- "Continuum models for dopant-defect evolution during excimer laser annealing in Silicon and Germanium materials", Department of Physics - University of Catania (July 2010).

7 Attended conferences

- "The 13th European Conference on Silicon Carbide and Related Materials" (ECSCRM 2020-2021) Vinci International Convention Centre (Palais des congrès), from October, Sunday 24th to Thursday 28th 2021, proudly hosted by the University of Tours. Poster: "Kinetics of surface instabilities and extended defects during the epitaxial growth of cubic silicon carbide".
- "2019 MRS Fall Meeting & Exhibit" December 1-6 2019 Boston, Massachusetts (USA). Oral presentation "Structure predictions in wet environments for ethanol and water adsorption on Anatase TiO2 (101) surfaces". Oral presentation "Role of evolving interface instabilities in the genesis and evolution of extended defects during epitaxil growth of cubic SiC". Poster "Why introducing Cs+ and MA+ cations in FAPbI3-based perovskites matters: an atomistic perspective"
- "FisMat Conference 2019", from 30/9 to 4/10 Department of Physics, Catania, Italy. Oral presentation "Structure predictions in wet environments for ethanol and water adsorption on Anatase TiO2 (101) surfaces". Oral presentation "Multiscale Ab-initio/Monte Carlo modelling for the growth kinetics of SiC substrates and nano-particles".
- "Spring Meeting of the European Materials Research Society (E-MRS)", 27-31/05/2019 Nice, France. Symposium X Silicon carbide and related materials for energy saving applications. Oral presentation "Ab-initio calibrated growth kinetics simulation of SiC substrates and nano-particles". Oral presentation "Structural and electronic properties of antiphase boundaries in 3C-SiC from first principles calculations".
- "Four Marvel Retreat" 07/09/2017, Lausanne, Switzerland. Poster presentation: "Soft-sphere continuum solvation in electronic structure calculations".
- "Coding Solvation Workshop" 23-25/08/2017, Livorno, Italy. Oral presentation: "Soft-sphere continuum solvation in electronic structure calculations".

- "Platform for Advanced Scientific Computing PASC 2017 Conference" 26-28/06/2017, Lugano, Switzerland. Poster presentation: "Soft-sphere continuum solvation in electronic structure calculations".
- "EMRS Spring Meeting Conference" 22-26/05/2017, Strasbourg, France. Poster presentation: "Complex wet-environments in electronic-structure calculations".
- "Platform for Advanced Scientific Computing PASC 2016 Conference" 8-10/06/2016, EPFL (Lausanne), Switzerland. Poster presentation: "Complex wet-environments in electronic-structure calculations"
- "APS March Meeting" 14-18/03/2016, Baltimora (USA). Oral presentation: "Complex wet-environments in electronic-structure calculations"
- "Psi-k Conference 2015" 06-10/09/2015, Donostia/San Sebastian, Spain. Oral presentation: G. Fisicaro et al. "A Generalized Poisson and Poisson-Boltzmann solver in wet-environments electronic-structure calculations" Symposium Electrochemical Energy Storage and Conversion: Solid/Liquid Interfaces.
- "Second Marvel Retreat" 03-04/09/2015, Lausanne, Switzerland. Poster presentation: G. Fisicaro et al. "A solver for the Generalized Poisson equation in wet-environments electronic-structure calculations".
- "Marvel Junior Retreat" 07-10/07/2015, Zurich, Switzerland. Oral presentation: G. Fisicaro et al. "A solver for the Generalized Poisson equation in wet-environments electronic-structure calculations".
- "Platform for Advanced Scientific Computing PASC 2015 Conference" 1-3/06/2015, Zurich, Switzerland. Poster presentation: G. Fisicaro et al. "A solver for the Generalized Poisson equation in wet-environments electronic-structure calculations".
- "ICTP Workshop on Advanced Quantum ESPRESSO Developer Training" 19-30/01/2015, Trieste, Italy. Poster: G. Fisicaro et al. "A generalized Poisson solver for complex electrostatic environments".
- "ICTP International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods" 15-17/01/2015, Trieste, Italy. Poster presentation: G. Fisicaro et al. "A generalized Poisson solver for complex electrostatic environments".
- ICMR workshop on "Ab-initio description of charged systems and solid/liquid interfaces forsemiconductors and electrochemisty", 6-11/07/2014, Santa Barbara (CA), USA. Oral presentation: G. Fisicaro et al. "Particle-particle interaction and space-dependent effective dielectric constant in colloidal system".
- "Platform for Advanced Scientific Computing PASC 2014 Conference" 2-3/06/2014, Zurich, Switzerland. Poster presentation: G. Fisicaro et al. "Particle-particle interaction and space-dependent effective dielectric constant in colloidal system".
- "E-MRS 2013 Spring meeting" from 27 to 31 May 2013 Strasburgo (France). Two oral presentations: G. Fisicaro et al "Boron activation and defects dynamics in Si solid-phase during excimer laser annealing processes" and "Boron redistribution and activation in silicon liquid phase under excimer laser irradiation" Symposium K, Physics and technology of advanced extra functionality CMOS-based devices.
- "18th International Conference on Simulation of Semiconductor Processes and Devices (SISPAD)" from 3 to 5 September 2013 Glasgow (Scotland). Oral presentation: G. Fisicaro et al. "Dopant dynamics and defects evolution in implanted silicon under laser irradiations: a coupled continuum and Kinetic Monte Carlo approach".
- "E-MRS 2012 Spring meeting" from 14 to 18 May 2012 Strasburgo (France). Oral presentaion: G. Fisicaro et al "Boron pile-up in implanted silicon induced by submicrosecond laser annealing"; Poster: "Kinetic Monte Carlo simulation of Phosphorous activation in implanted Siliconby submicrosecond laser thermal annealing" Symposium A, Advanced Silicon Materials Research for Electronic and Photovoltaic Applications III.

- "19th International Conference on Ion Implantation Technology" from 25 to 29 June 2012 Valladolid (Spain). Oral presentation: G. Fisicaro et al "Kinetic Monte Carlo simulation of dopant-defect systems under submicrosecond laser thermal processes"; Poster: "Dynamics of dopant redistribution in molten Silicon caused by laser irradiation".
- "E-MRS 2011 Spring meeting IUMRS ICAM 2011 & E-MRS/MRS Bilateral conferenceon energy" from 9 to 13 May 2011 Nice (France). Oral presentation: G. Fisicaro et al "Excimer laser annealing of Phosphorous implanted Silicon: experimental analysis and modeling" Symposium J, Laser materials processing for micro and nano applications.
- "12th International Symposium on Laser Precision Microfabrication" Takamatsu (Japan) from 7 to 10 June 2011. Oral presentation: G. Fisicaro et al "Dopant activation modeling in implanted Silicon under multi-pulsed excimer laser irradiation" section Micromachining and Modification.
- "E-MRS 2010 Spring Meeting" from 7 to 11 June 2010 at the Congress Center-Place de Bordeaux, Wacken, Strasbourg, France. Two oral presentations: G. Fisicaro et al "Dopant activation and damage evolution in implanted Silicon after Excimer Laser Annealing" and Symposium I, Advanced silicon materials research for electronic and photovoltaic applications; G. Fisicaro et al "Laser annealing doping processes of SiGe and Ge based devices". Symposium H, Post-Si CMOS electronic devices: the role of Ge and III-V materials.
- "XCVI Congress of the Italian Physics Society" 20-24/09/2010, Bologna. Oral presentation: G. Fisicaro et al "Dopant activation and damage evolution in implanted silicon by pulsed excimer laser annealing." Section II, Material science.
- "17th IEEE International Conference on Advanced Thermal Processing of Semiconductors - RTP 2009" from 29 September to 2 October 2009 Marriott Hotel Albany-NY. Oral presentation: G. Fisicaro et al "Damage Evolution in Implanted Silicon by Pulsed Excimer Laser Annealing".

8 Attended workshops

- "School of the 19th International Conference on Ion Implantation Technology", from 21 to 23 June 2012 Valladolid (Spain).
- "Carbomat,international workshop on Carbon-based Low Dimensional Materials", 5-7 December 2011, at the CNR-IMM Catania.
- "35th Workshop on Compound Semiconductor Devices and Integrated Circuits, WOCSDICE 2011", from 29 May to 1 June 2011, at the CNR-IMM Catania.
- "Carbomat,international workshop on Carbon-based Low Dimensional Materials", 6-8 October 2010, at the CNR-IMM Catania.
- "Challenges in Material Science", 26 May 2010 Department of Physics - University of Catania.

9 Teaching activities

Teaching assistant for the following courses held at the Physics Department, University of Basel:

- Computational Physics, exercitation class and Fortran tutorial (from 01/10/2014 to 31/12/2014);
- Electronic-structure calculations, exercitation class (from 01/03/2015 to 31/04/2015);
- Global structure predictions, exercitation class (from 01/04/2015 to 30/04/2015);
- Computational Physics, exercitation class and Fortran tutorial (from 01/10/2015 to 31/12/2015);
- Global structure predictions, exercitation class (from 01/03/2016 to 30/03/2016);
- Computational Physics, exercitation class and Fortran tutorial (from 01/10/2016 to 31/12/2016);
- Computational Physics, exercitation class and Fortran tutorial (from 01/10/2017 to 31/12/2017);

10 Project participation

- Principal Investigator for the computational project "Effects of complex liquid environments on material properties", a computational project for node/hours at the Swiss National Supercomputing Center (CSCS) Switzerland under Project ID s869. Computational hours 800 000 node hours (9 600 000 cpu hours) on Daint HPC machine from 1 October 2018 to 30 September 2020. Projects: Many important physicochemical processes take place in solution, both in the context of basic as well as industrial research. Here we aim at developing and assessing a groundbreaking theoretical/computational paradigm to study complex wet environment effects on material properties at an atomistic level. Since material properties are ultimately related to the underlying atomic structure, we plan to extend current ab-initio structure prediction codes to wet environments. Solvents will be described by a recently developed implicit solvation model, called "soft-sphere". The approach aims at overcoming all drawbacks that hinder the application of structure predictions to wet environments. Among them, the explosion of the system size when explicit solvent molecules are considered, which makes simulations extremely costly from a computational point of view. A first application of the proposed computational paradigm has been demonstrated successful at describing surface reconstructions of fluorite in water. The methodology will be benchmarked with target experiments and molecular dynamics simulations. Molecular doping of silicon, small TiO2 clusters, and surfaces in various solvents will be some of the systems to be investigated. Target experiments will be carried out by the applicant partner CNR-IMM in Catania, Italy. Here we suggest a two-year project with a total of 800000 node hours, for which we would like to have an allocation of 400000 node hours in the first year.

- Participation as researcher to the research activity of the H2020 European Project Mundfab "Modeling Unconventional Nanoscaled Device FABrication" Grant Agreement No. 871813. For the last 50 years, shrinking transistors have enabled more and more processing capacity to be put on the same size chips, following Intel co-founder Gordon Moore's predictions in the 1960s. Moore's law is reaching its physical and economic limits – our future virtually unlimited interconnectedness will depend on a paradigm shift. Much as high-rises are a solution to urban growth, emerging 3D sequential integration could alleviate the problems faced by 2D CMOS transistor technology. Bringing this architecture down to the nanoscale could additionally enhance the already sizeable benefits. Building on extensive experimental work and data, the EU-funded MUNDFAB project is developing the requisite modelling and simulation tools that will foster innovation via virtual fabrication of the next generation of nanoscale electronic devices. Project start 1 January 2020, End 31 December 2022 at CNR Institute for Microelectronics and Microsystems (Catania, Italy).

- Participation as researcher to the research activity of the H2020 European Project CHALLENGE "3C-SiC Hetero-epitaxiALLy grown on silicon compliancE substrates and 3C- SiC substrates for sustaiNable wide-band-Gap powEr devices" HORIZON 2020-NMBP- 720827. Within CHALLENGE a new approach is proposed to improve the quality and to reduce stress: it is necessary to modify the structure of the substrate (compliance substrate) in order to force the system to reduce the defects while increasing the thickness of the layer. Furthermore, by using the typical bulk growth techniques used for 4H-SiC it is possible to grow bulk 3C-SiC wafers, improving considerably the quality of the material. Project start 1 January 2017, End 30 June 2020 at CNR Institute for Microelectronics and Microsystems (Catania, Italy).

- Participation as researcher to the research activity of the European Project Best4U "Bifacial, high efficiency 4-terminals solar cell technology for utility scale" The Best4U project focuses on industrial research aimed at finding solutions to increase the efficiency of photovoltaic modules by more than 25% and improve bi-faciality, because this reduces significantly both the associated BOS and LCOE. To obtain this improvement in efficiency and productivity, the concept of a 4-terminal photovoltaic module is proposed. 4T cells and modules can be considered as an alternative to tandem photovoltaic cells with some important advantages. The conventional monolithic tandem cell connected in series in fact is limited by the necessity of matching the lattice parameter and current of the 2 cells in series. On the contrary, the 4-terminal structure is not affected by these aspects and this adds considerable degrees of freedom. The present proposal therefore has as its objective the realization of a 4-terminal cell / module in which the lower cell is a double-sided heterojunction Si cell, and the upper cell is a wide band-gap semiconductor cell. the double-sided lower part collects and transforms the incident red and infrared light

passing through the top cell into electricity, and the albedo light reflected / diffused from the ground from the rear. The first cell collects and transforms the blue portion of the incident solar spectrum. The goal is an efficiency in standard conditions greater than 25%. For this purpose, some approaches will be studied in parallel and compared, and the most promising will be defined. A double-sided photovoltaic field demonstrator optimized for the exploitation of the albedo of the soil with a productivity in kWh / kWp greater than 20% compared to the single-sided system will also be created. Project start 1 April 2020, End 1 October 2022 at CNR Institute for Microelectronics and Microsystems (Catania, Italy).

- Participation as researcher to the Swiss NCCR MARVEL project (http://nccr-marvel.ch), which represents a centre on Computational Design and Discovery of Novel Materials, that has been created by the Swiss National Science Foundation in May 2014. The goal of the NCCR MARVEL is to radically transform and accelerate invention and discovery in science and technology, and especially to transform and accelerate the design and discovery of novel materials in order to achieve improved properties and performance, or to witness the emergence of original physical properties. We will achieve this goal by exploiting the predictive accuracy that quantum-mechanical simulations have now reached for realistic, complex systems, the treasure trove of ever-increasing computational power ideally suited to intrinsically parallel problems, and the powerful synergies arising with the computer science of heterogeneous data management, data mining, and machine learning. EPFL acts as the leading house, and it is directed by Nicola Marzari, but it involves 41 principal investigators across 12 Swiss Institutions: the two Federal Institutes of Technology in Lausanne and Zurich (EPFL and ETHZ), six universities in Basel, Bern, Fribourg, Geneva, Svizzera Italiana, and Zurich (UNIBAS, UNIBE, UNIFR, UNIGE, USI, UZH), the Swiss National Supercomputing Centre (CSCS), the research laboratories of IBM Zurich, the two federal research institutes, the Paul Scherrer Institute (PSI), and the Swiss Federal Laboratories for Materials Science and Technology (Empa). The applicant integrated his research in Basel to the various work-packages of the Marvel project.

- Participation as main researcher to the Swiss PASC project "ENVIRON: A Library for Complex Electrostatic Environments in Electronic- structure Simulations" at the Department of Physics, University of Basel from 17 March 2014. The project is in collaboration with Prof. Dr. Nicola Marzari Theory and Simulation of Mate- rials Institute of Materials EPFL, Lausanne and Prof. Dr. Juerg Hutter Physics Department University of Zurich. The applicant cared the development of a library to include complex wet environments in electronic-structure calculations. Development, parametrization and test of implicit solvation models for neutral and ionic solvents (http://www.quantum-environment.org).

- Participation as researcher to the research activity of the European Project "Advanced Technology Modeling for Extra-Functionality Devices – Enlarged EU ATEMOX" Grant Agrement N 287669 from 15/01/2012 to 16/03/2014 (https://www.atemox.eu). To reach the ambitious goals, a consortium of European companies active in complementary fields of competence (STMicroelectronics: device manufacturing, Synopsys: TCAD software, Exico, IBS: equipment production, Probion, Semilab: characterization) and leading European research institutes (CNRS-LAAS/CEMES, CNR-IMM, ETH-Zurich, Fraunhofer-IISB, Univ. Newcastle) has been formed to expertly cover all fields from experiment via characterization and modelling to simulation as well as to ensure full coverage of the value chain. In particular, the applicant tackled the study of dopant-defects evolution during thermal laser annealing processes by means of continuum models and kinetic Monte Carlo simulations.

11 Software developments

- BigDFT software package (https://bigdft.org). BigDFT is a DFT massively parallel electronic structure code (GPL license) using a wavelet basis set. Wavelets form a real space basis set distributed on an adaptive mesh (two levels of resolution in our implementation). GTH or HGH pseudopotentials are used to remove the core electrons. Thanks to our Poisson solver based on a Green function formalism, periodic systems, surfaces and isolated systems can be simulated with the proper boundary conditions.

- MulSKIPS, a Kinetic Monte Carlo super-Lattice code, designed to study with an atomic resolution the growth kinetics of elements, alloys and compounds characterized by the sp3 bond

symmetry.

- ENVIRON: A Library for Complex Electrostatic Environments in Electronic-structure Simulations (http://www.quantum-environ.org) Environ is a computational library aimed at introducing environment effects into atomistic first-principles simulations, in particular for applications in surface science and materials design. A hierarchical, multi-scale, strategy is at the base of the different methods implemented: while the atomistic and electronic details of the system of interest are fully preserved, the degrees of freedom of the surrounding environment (being it a liquid solution of a more complex embedding) are treated using simplified approaches. By reducing the number of degrees of freedom and by exploiting intrinsic or faster statistical averaging, the implemented methods allow the systematic un-expensive study of large systems.