



Ioannis Deretzis

Date of birth: 22/09/1976 | **Nationality:** Greek | **Gender:** Male | (+39) 0955968321 |

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Institute for Microelectronics and Microsystems, Z.I. VIII strada 5, 95121, Catania, Italy

● WORK EXPERIENCE

26/11/2012 – CURRENT – Catania, Italy

RESEARCHER – CNR INSTITUTE FOR MICROELECTRONICS AND MICROSYSTEMS

- Computational materials science
- Density functional theory
- Classical and *ab initio* molecular dynamics
- Quantum transport and device modeling
- Simulations of experimental techniques
- Hybrid perovskites, low-dimensional materials, materials for microelectronics and energy

03/01/2011 – 25/11/2012 – Catania, Italy

POST-DOC RESEARCH FELLOW – CNR INSTITUTE FOR MICROELECTRONICS AND MICROSYSTEMS

- Computational study of low-dimensional systems
- Development of computational codes for materials science

01/03/2004 – 05/03/2008 – Catania, Italy

RESEARCH COLLABORATOR – CNR INSTITUTE FOR MICROELECTRONICS AND MICROSYSTEMS

- Development of computational codes for materials science

● EDUCATION AND TRAINING

01/01/2008 – 16/12/2010 – Italy

DOCTOR OF PHILOSOPHY (PHD) IN NANOSCIENCE – University of Catania

01/09/2000 – 11/07/2002 – United Kingdom

MASTER OF SCIENCE (MSC) IN MUSIC TECHNOLOGY – University of York

30/09/1994 – 20/03/2000 – Greece

DEGREE IN PHYSICS – Aristotle University of Thessaloniki

● LANGUAGE SKILLS

Mother tongue(s): **GREEK**

Other language(s):

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken production	Spoken interaction	
ENGLISH	C2	C2	C2	C2	C2
ITALIAN	C2	C2	C2	C2	C2

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

● PUBLICATIONS

Exploring the Structural Competition between the Black and the Yellow Phase of CsPbI₃

Nanomaterials 2021, 11(5), 1282
<https://doi.org/10.3390/nano11051282> – 2021

Genesis and evolution of extended defects: The role of evolving interface instabilities in cubic SiC

Applied Physics Reviews 7, 021402 (2020)
<https://doi.org/10.1063/1.5132300> – 2020

Temperature-Dependent Optical Band Gap in CsPbBr₃, MAPbBr₃, and FAPbBr₃ Single Crystals

J. Phys. Chem. Lett. 2020, 11, 7, 2490–2496
<https://doi.org/10.1021/acs.jpclett.0c00295> – 2020

Local Order and Rotational Dynamics in Mixed A-Cation Lead Iodide Perovskites

J. Phys. Chem. Lett. 2020, 11, 3, 1068–1074
<https://doi.org/10.1021/acs.jpclett.9b03763> – 2020

Pb clustering and PbI₂ nanofragmentation during methylammonium lead iodide perovskite degradation

Nature Communications 10, 2196 (2019)
<https://doi.org/10.1038/s41467-019-09909-0> – 2019

Nitrogen Soaking Promotes Lattice Recovery in Polycrystalline Hybrid Perovskites

Adv. Energy Mater. 2019, 9, 1803450
<https://doi.org/10.1002/aenm.201803450> – 2019

Stability and Degradation in Hybrid Perovskites: Is the Glass Half-Empty or Half-Full?

J. Phys. Chem. Lett. 2018, 9, 11, 3000–3007
<https://doi.org/10.1021/acs.jpclett.8b00120> – 2018

Exploring the orthorhombic–tetragonal phase transition in CH₃NH₃PbI₃: the role of atom kinetics

Nanoscale, 2017, 9, 5896–5903
<https://doi.org/10.1039/C7NR01818E> – 2017

Spontaneous bidirectional ordering of CH₃NH₃⁺ in lead iodide perovskites at room temperature: The origins of the tetragonal phase

Scientific Reports 6, 24443 (2016)
<https://doi.org/10.1038/srep24443> – 2016

Stability of solution-processed MAPbI₃ and FAPbI₃ layers

Phys. Chem. Chem. Phys., 2016, 18, 13413–13422
<https://doi.org/10.1039/C6CP00721J> – 2016

Atomistic origins of CH₃NH₃PbI₃ degradation to PbI₂ in vacuum

Appl. Phys. Lett. 106, 131904 (2015)
<https://doi.org/10.1063/1.4916821> – 2015

Origin and impact of sublattice symmetry breaking in nitrogen-doped graphene

Phys. Rev. B 89, 115408 (2014)
<https://doi.org/10.1103/PhysRevB.89.115408> – 2014

Direct growth of quasi-free-standing epitaxial graphene on nonpolar SiC surfaces

Phys. Rev. B 88, 085408 (2013)
<https://doi.org/10.1103/PhysRevB.88.085408> – 2013

Delaminated Graphene at Silicon Carbide Facets: Atomic Scale Imaging and Spectroscopy

ACS Nano 2013, 7, 4, 3045–3052
<https://doi.org/10.1021/nn305922u> – 2013

Electronic transport at monolayer-bilayer junctions in epitaxial graphene on SiC

Phys. Rev. B 86, 235422 (2012)
<https://doi.org/10.1103/PhysRevB.86.235422> – 2012

Role of covalent and metallic intercalation on the electronic properties of epitaxial graphene on SiC(0001)

Phys. Rev. B 84, 235426 (2011)
<https://doi.org/10.1103/PhysRevB.84.235426> – 2011

Effects due to backscattering and pseudogap features in graphene nanoribbons with single vacancies

Phys. Rev. B 81, 085427 (2010)
<https://doi.org/10.1103/PhysRevB.81.085427> – 2010

Phonon Driven Nonlinear Electrical Behavior in Molecular Devices

Phys. Rev. Lett. 99, 136404 (2007)
<https://doi.org/10.1103/PhysRevLett.99.136404> – 2007

Role of contact bonding on electronic transport in metal-carbon nanotube-metal systems

Nanotechnology 17 5063
<https://doi.org/10.1088/0957-4484/17/20/005> – 2006

● PROJECTS

01/01/2020 – CURRENT

Modeling Unconventional Nanoscaled Device FABrication (MUNDFAB)

Type: Horizon 2020 project. Role: Deputy Partner Representative

19/08/2019 – 19/08/2020

Structure Prediction, Kinetic Evolution and Carrier Transport in Hybrid Perovskites for Solar Cell Applications (HYPER SOL)

Type: ISCRA-CINECA Class B computational project. Role: Principal Investigator

09/08/2017 – 09/05/2018

Large-scale ab initio molecular dynamics simulations for the stability of hybrid perovskite solar cells (MD-HYPER)

Type: ISCRA-CINECA Class C computational project. Role: Principal Investigator

19/12/2011 – 19/02/2013

Ab initio quantum transport simulations of substrate-supported graphene (SUBGRAPH)

Type: ISCRA-CINECA Class C computational project. Role: Principal Investigator

01/04/2019 – CURRENT

Metrology Advances for Digitized ECS industry 4.0 (MADEin4)

Type: Horizon 2020 project. Role: Participant

01/01/2017 – 30/06/2021

3C-SiC Hetero-epitaxiALLY grown on silicon complianceE substrates and 3C-SiC substrates for sustaiNable wide-band-Gap powEr devices (CHALLENGE)

Type: Horizon 2020 project. Role: Participant

01/02/2016 – 30/01/2019

Graphene heterostructures with Nitrides for high frequency Electronics (GraNitE)

Type: FLAG-ERA Joint Transnational Call. Role: Participant

26/11/2012 – 31/12/2013

Graphene on SiC wafers for high performance RF transistors (GRAPHIC-RF)

Type: European Science Foundation (ESF), EuroGRAPHENE. Role: Participant

● OTHER INFORMATION

Metrics

- Number of publications: 105
- H-index: 24 (Scopus)
- Number of citations: 1733 (Scopus)

Reviewer activity

Reviewer for

- Energy & Environmental Science
- Advanced Materials
- Advanced Energy Materials
- ACS Nano
- Applied Physics Letters
- Journal of the American Chemical Society
- Journal of Physical Chemistry Letters
- Journal of Materials Chemistry A
- Nanoscale
- Nanotechnology
- Scientific Reports

Invited talks

- 'Electron quantum transport in disordered graphene', CIMTEC 2014 - 13th International Conference on Modern Materials and Technologies.
- 'Introduction to DFT modeling for EELS simulations', 1st Italian EELS school, 2014
- 'Theory and process simulation of epitaxial graphene on SiC', Workshop on the Science and Applications of Epitaxial Graphene on SiC (EPIGRAPHIC), 2012

Teaching

- 'Quantum-mechanical derivation methods for the simulation of complex systems', Scuola Superiore, University of Catania, 2019-2020
- 'Computational Complexity Course', Scuola Superiore, University of Catania, 2012-2013