EMILIO SCALISE

Surname: Scalise **Name**: Emilio

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Date of birth: 06.11.1985 **Place of Birth**: Crotone (Italy)
Nationality: Italian **Marital Status**: Married

EDUCATION

2009-2013 **Ph.D. Researcher in Physics (Semiconductor Physics),**
University of Leuven (Belgium).
Field of study: First-principles modeling of structural, vibrational and electronic properties of high-k dielectrics/high-mobility semiconductors heterostructures and (quasi) 2D materials.

2007–2009 **Master of Electronic Engineering**,
University of Calabria (Italy).
Final degree mark: 110 (out of 110) cum laude
Graduation date: 22/09/2009
Official time limit for the degree course: 2 years
Dissertation/thesis title:
FIRST - PRINCIPLES MODELING OF DEFECTS IN GE MOS DEVICES
Months needed to complete the thesis/dissertation: 6
Number of exams taken abroad: 8
Institution/company/organization where traineeship/internship has been carried out: IMEC, Belgium.

2004-2007 **Bachelor of Electronic Engineering**,
University of Calabria (Italy).
Dissertation: Design of a home automation system by power line communication.
Final degree mark: 110 (out of 110).

1999-2004 **Scientific School** (secondary school)
Liceo scientifico Filolao, Crotone (Italy).
Final degree mark: 100 (out of 100).

PROFESSIONAL POSITIONS

11.2017-present: **Research Fellow.**
Department of Materials Science, University of Milano Bicocca, 20152 Milan, Italy

02.2014-10.2017: **Post-doc Researcher**.
Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

12.2009-01/2014: **Researcher**.
K.U. Leuven, Semiconductor Physics Section, Celestijnenlaan 200d
3001 Leuven, Belgium

02.2009-09.2009: **Trainee**.
IMEC, Kapeldreef, 75
3001 Leuven, Belgium.

FELLOWSHIPS AND AWARDS

2017-2020 Research fellow (RtdA), Department of Materials science, University of Milano Bicocca, Italy
2013 EMRS Young Scientist Award
2015 Nano Research 2012 top papers award
2015 Nano Research 2013 top papers award
2016 Top Cited Article 2014-2015 in 2D Materials
2013 Outstanding Ph.D. thesis at the University of Leuven (Belgium) and publication in the "Springer Theses", special series recognizing outstanding Ph.D. research.

TEACHING SKILLS

2019 National habilitation to academic professorship:
"Abilitazione Scientifica Nazionale a professore di II fascia"
2018 – pres. Teaching assistant and Lecturer- University of Milano Bicocca (Unimib), IT
2011 – 2013 Teaching assistant - KULeuven, BE (see Appendix)

SUPERVISION OF GRADUATE STUDENTS

2018 – 2019 Supervision of Master Students (M. Loda, F. Grassi, A. Carbone)
Department of Physics, University of Milano Bicocca, Italy
2012 – 2013 Supervisor – Project Work Nanoscience (Master in Physics), KULeuven, BE

INSTITUTIONAL RESPONSIBILITIES

2018 – 2019 Faculty member, University of Milano Bicocca, Italy
2018 – 2019 Member of the selection board for postdoctoral fellowships, Department of Materials Science, University of Milano Bicocca, Italy
2018 – 2019 Member of the Master thesis dissertation committee, Physics and Materials Science Departments, University of Milano Bicocca, Italy

REVIEWING ACTIVITIES

2018 Reviewer for a scientific project funded by the Basic Energy Sciences (BES) program of the U.S. Department of Energy, Science Office.
as of today Reviewer for different scientific Journals, including (recent): Chemical Society Reviews (tracked in Publons), the Journal of Physical Chemistry Letters, Applied Surface Science
2018 – 2019 Master thesis reviewer, Physics Department, University of Milano Bicocca, Italy

MEMBERSHIPS OF SCIENTIFIC SOCIETIES

2015 – pres. American Physical Society

POSTGRADUATE SCHOOLS

2012 Training course: “Nanometer CMOS ICs”, IMEC, Belgium

2011 CECAM Tutorial “Computational spectroscopy using Quantum Espresso and related codes”, SISSA, Trieste, Italy

2010 “School on Computational Modelling of Materials”, University of Antwerp, Belgium

TECHNICAL SKILLS

- Expert in modeling of structural, vibrational, electronic and interface properties of materials for semiconductor based applications, particularly in the field of Density Functional Theory and beyond, including hybrid functional (pbe0, HSE), GW approximation and linear-response techniques.
- Expert in modeling and simulation of (quasi) 2D materials, nanoparticles, material interfaces and surfaces.
- Theoretical Knowledge in electrical measurements for nanoelectronic devices and semiconductor characterization techniques
- Development and implementation of state-of-the art modelling approaches based on modern physics and chemistry concepts.
- Expertise in electronic structure codes (Quantum Espresso, VASP, abinit, SIESTA)
- Authors of several publications in international referee journals (see Appendix).

INFORMATIC SKILLS

- Programming languages: C++,Fortran, Basic, Visual Basic and Python(notions).
- Shell Scripting, Administration and management of UNIX/LINUX and Windows file systems(Basic).
- Creation and management of simple web sites.
- Practice of the office suite (Word, Excel, PowerPoint,…), Matlab and Labview.

LINGUISTIC SKILLS

- **Italian** Mother Tongue.
- **English** Spoken, read and written. Fluent.
- **German** Spoken, read and written. Level: Intermediate.
- **Dutch** Read and written. Level: Limited.

MISCELLANEOUS

- Leisure: informatics, fitness, reading, cinema.
- Driving license B.

Appendix: publications, teaching and research activities

Teaching activities

Courses of study	Course	Teaching hours	Activities	Academic years
Bachelor in Materials Science	STRUTTURA DELLA MATERIA II	24	Exercises and Lectures	2019/2020
Bachelor in Chemical Science and Technology	FISICA II	24	Exercises	2018/2019 2019/2020
Bachelor in Materials Science	FISICA II	12	Exercises	2017/2018
Master in Physics	LABORATORIO DI STATO SOLIDO ED ELETTRONICA II	36	Laboratory sessions	2018/2019
Master in Materials Science	TERMODINAMICA STATISTICA DEI MATERIALI	24	Laboratory sessions	2017/2018
Bachelor in Physics	PHYSICS: Mechanics	16	Exercises	2011/2012 2012/2013

Submitted research projects (with evaluation)

- CINECA HPC: **Class B ISCRA project**.
  Title: *Multiscale mOdelling of 3C-SiC Hetero-Epitaxy: integrating atomistic and continiumm modelling (MOCHE)*
  Duration: from 30/07/2018 to 30/07/2019
  Role: Principal Investigator
  Result: 1.4 million CPUhs granted
- CINECA HPC: **Class C ISCRA project**.
  Title: *Sn incorporation In Ge/GeSn core/shell Nanowires: a first-principles study (SIGN)*
  Duration: from 11/18/2018 to 11/07/2019
  Role: Principal Investigator
  Result: 500k CPUhs granted
- CINECA HPC: **Class B ISCRA project**.
  Title: *hExagonal cRystals of Germanium and silicOn (ERGO)*
  Duration: from 29/04/2020 to 29/04/2021
  Role: Principal Investigator
  Result: 1.5 million CPUhs granted
- ERC: **ERC Starting Grant project**.

Title: *Hexagonal allotropes for group IV photonics (HEXATROPES4)*
Duration: 60 months **Requested Budget**:1.435.000 Euros
Submission date: October 2019
Role: Principal Investigator
Result
Final Score: B (the project is of high quality but not sufficient to pass to Step 2 of the evaluation)
Ranking range*: 37%-46% (only the top 36% of the proposals evaluated in panel PE5 were retained for Step 2.)

Participation in international projects

I have been working in three different international research projects and in three different countries in Europe, both in academic and non-academic institutions, contributing to several reports and review of these projects:

06.2011-12.2013
Participation in the project "2DNANOLATTICES" within the "7th Framework Program of the European Commission –Future and Emerging Technologies (FET)". Most of my PhD work has been conducted within this project.

02.2014-10.2017
Participation in the research project granted by the German research ministry within the "NanoMatFutur" programme. A fruitful cooperation between my group (Atomistic Modelling group) at the Max Planck Institute and other international research group, particularly the at the University of Chicago, has been possible thanks to this project.

11.2017-pres.
I conduct part of the work contributing with my current group to the EU research project CHALLENGE, which is a HORIZON 2020 project devoted to the study of cubic silicon carbide (3C-SiC) and involving both academic and industrial partners.

Articles in internationally reviewed academic journals:

- Muckel, F.; Lorenz, S.; Yang, J.; Nugraha, T. A.; Scalise, E.; Hyeon, T.; Wippermann, S.; Bacher, G. Exciton-Driven Change of Phonon Modes Causes Strong Temperature Dependent Bandgap Shift in Nanoclusters. *Nat. Commun.* **2020**. DOI:10.1038/s41467-020-17563-0.
- Scalise, E.; Barbisan, L.; Sarikov, A.; Montalenti, F.; Miglio, L.; Marzegalli, A. The Origin and Nature of Killer Defects in 3C-SiC for Power Electronic Applications by a Multiscale Atomistic Approach. *J. Mater. Chem. C* **2020**, *8* (25), 8380–8392. DOI:10.1039/D0TC00909A.
- Scalise, E. Tailoring the Electronic Properties of Semiconducting Nanocrystal-Solids. *Semiconductor Science and Technology*. 2020. DOI:10.1088/1361-6641/ab52e0.
- Molle, A.; Faraone, G.; Lamperti, A.; Chiappe, D.; Cinquanta, E.; Martella, C.; Bonera, E.; Scalise, E.; Grazianetti, C. Stability and Universal Encapsulation of Epitaxial Xenes. *Faraday Discuss.* **2020**. DOI:10.1039/C9FD00121B.
- Sarikov, A.; Marzegalli, A.; Barbisan, L.; Scalise, E.; Montalenti, F.; Miglio, L. Molecular Dynamics Simulations of Extended Defects and Their Evolution in 3C–SiC by Different Potentials. *Model. Simul. Mater. Sci. Eng.* **2020**, *28* (1), 015002. DOI:10.1088/1361-651X/ab50c7.
- Assali, S.; Bergamaschini, R.; Scalise, E.; Verheijen, M. A.; Albani, M.; Dijkstra, A.; Li, A.; Koelling, S.; Bakkers, E. P. A. M.; Montalenti, F.; Miglio, L. Kinetic Control of Morphology and

Composition in Ge/GeSn Core/Shell Nanowires. *ACS Nano* **2020**, *14* (2), 2445–2455. DOI:10.1021/acsnano.9b09929.

- Scalise, E.; Marzegalli, A.; Montalenti, F.; Miglio, L. Temperature-Dependent Stability of Polytypes and Stacking Faults in SiC: Reconciling Theory and Experiments. *Phys. Rev. Appl.* **2019**, *12* (2), 021002. DOI:10.1103/PhysRevApplied.12.021002.
- Scalise, E.; Srivastava, V.; Janke, E.; Talapin, D.; Galli, G.; Wippermann, S. Surface Chemistry and Buried Interfaces in All-Inorganic Nanocrystalline Solids. *Nat. Nanotechnol.* **2018**, *13* (9), 841–848. DOI:10.1038/s41565-018-0189-9.
- Scalise, E.; Iordanidou, K.; Afanas'ev, V. V.; Stesmans, A.; Houssa, M. Silicene on Non-Metallic Substrates: Recent Theoretical and Experimental Advances. *Nano Res.* **2018**, *11* (3), 1169–1182. DOI:10.1007/s12274-017-1777-y.
- Scalise, E.; Houssa, M. Predicting 2D Silicon Allotropes on SnS_2. *Nano Res.* **2017**, *10* (5), 1697–1709. DOI:10.1007/s12274-016-1409-y.
- van den Broek, B.; Houssa, M.; Scalise, E.; Pourtois, G.; Afanas'ev, V. V; Stesmans, A. First-Principles Electronic Functionalization of Silicene and Germanene by Adatom Chemisorption. *Appl. Surf. Sci.* **2014**, *291*, 104–108. DOI:10.1016/j.apsusc.2013.09.032.
- Broek, B. van den; Houssa, M.; Scalise, E.; Pourtois, G.; Afanas'ev, V. V; Stesmans, A. Two-Dimensional Hexagonal Tin: *Ab Initio* Geometry, Stability, Electronic Structure and Functionalization. *2D Mater.* **2014**, *1* (2), 021004. DOI:10.1088/2053-1583/1/2/021004.
- Scalise, E.; Cinquanta, E.; Houssa, M.; van den Broek, B.; Chiappe, D.; Grazianetti, C.; Pourtois, G.; Ealet, B.; Molle, A.; Fanciulli, M.; Afanas'ev, V. V; Stesmans, A. Vibrational Properties of Epitaxial Silicene Layers on (111) Ag. *Appl. Surf. Sci.* **2014**, *291*, 113–117. DOI:10.1016/j.apsusc.2013.08.113.
- Scalise, E.; Houssa, M.; Cinquanta, E.; Grazianetti, C.; Van Den Broek, B.; Pourtois, G.; Stesmans, A.; Fanciulli, M.; Molle, A. Engineering the Electronic Properties of Silicene by Tuning the Composition of MoX_2 and GaX (X=S,Se,Te) Chalchogenide Templates. *2D Mater.* **2014**, *1* (1), 1–11. DOI:10.1088/2053-1583/1/1/011010.
- Scalise, E.; Cinquanta, E.; Houssa, M.; van den Broek, B.; Chiappe, D.; Grazianetti, C.; Pourtois, G.; Ealet, B.; Molle, A.; Fanciulli, M.; Afanas'ev, V. V.; Stesmans, A. Vibrational Properties of Epitaxial Silicene Layers on (111) Ag. *Appl. Surf. Sci.* **2014**, *291*, 113–117. DOI:10.1016/J.APSUSC.2013.08.113.
- Cinquanta, E.; Scalise, E.; Chiappe, D.; Grazianetti, C.; van den Broek, B.; Houssa, M.; Fanciulli, M.; Molle, A. Getting through the Nature of Silicene: An Sp^2 –Sp^3 Two-Dimensional Silicon Nanosheet. *J. Phys. Chem. C* **2013**, *117* (32), 16719–16724. DOI:10.1021/jp405642g.
- Houssa, M.; Van Den Broek, B.; Scalise, E.; Ealet, B.; Pourtois, G.; Chiappe, D.; Cinquanta, E.; Grazianetti, C.; Fanciulli, M.; Molle, A.; Afanas'Ev, V. V.; Stesmans, A. Theoretical Aspects of Graphene-like Group IV Semiconductors. *Appl. Surf. Sci.* **2014**, *291*, 98–103. DOI:10.1016/j.apsusc.2013.09.062.
- Houssa, M.; van den Broek, B.; Scalise, E.; Pourtois, G.; Afanas'ev, V. V.; Stesmans, A. An Electric Field Tunable Energy Band Gap at Silicene/(0001) ZnS Interfaces. *Phys. Chem. Chem. Phys.* **2013**, *15* (11), 3702. DOI:10.1039/c3cp50391g.
- Scalise, E.; Houssa, M.; Pourtois, G.; van den Broek, B.; Afanas'ev, V.; Stesmans, A. Vibrational Properties of Silicene and Germanene. *Nano Res.* **2013**, *6* (1), 19–28. DOI:10.1007/s12274-012-0277-3.
- Scalise, E.; Houssa, M.; Pourtois, G.; Afanasev, V. V.; Stesmans, A. First-Principles Study of Strained 2D MoS_2. *Phys. E Low-Dimensional Syst. Nanostructures* **2014**, *56*, 416–421. DOI:10.1016/j.physe.2012.07.029.

- Scalise, E.; Houssa, M.; Pourtois, G.; Afanas'ev, V.; Stesmans, A. Strain-Induced Semiconductor to Metal Transition in the Two-Dimensional Honeycomb Structure of MoS_2. *Nano Res.* **2012**, *5* (1), 43–48. DOI:10.1007/s12274-011-0183-0.
- Scalise, E.; Houssa, M.; Pourtois, G.; Afanas'ev, V. V.; Stesmans, A. Inelastic Electron Tunneling Spectroscopy of HfO_2 Gate Stacks: A Study Based on First-Principles Modeling. *Appl. Phys. Lett.* **2011**, *99* (13), 132101. DOI:10.1063/1.3644158.
- Houssa, M.; Scalise, E.; Sankaran, K.; Pourtois, G.; Afanas'ev, V. V.; Stesmans, A. Electronic Properties of Hydrogenated Silicene and Germanene. *Appl. Phys. Lett.* **2011**, *98* (22), 223107. DOI:10.1063/1.3595682.
- Scalise, E.; Houssa, M.; Pourtois, G.; Afanas'ev, V. V.; Stesmans, a. Structural and Vibrational Properties of Amorphous GeO_2 from First-Principles. *Appl. Phys. Lett.* **2011**, *98* (20), 202110. DOI:10.1063/1.3593036.

Books

- E. Scalise, Theoretical study of transition metal dichalcogenides, chapter in "2D Materials for Nanoelectronics" edited by M. Houssa, A. Dimoulas, A. Molle. Edition: Series in Materials Science and Engineering, Publisher: CRC Press (Taylor & Francis), ISBN: 9781498704175 (2016).
- E. Scalise, Vibrational Properties of Defective Oxides and 2D Nanolattices: Insights from first-principles simulations. *Springer Theses* (2014).

Proceedings Paper

- M. Houssa, E. Scalise, B. van den Broek, A. Lu, G. Pourtois, V. V. Afanas'ev and A. Stesmans, Interaction of silicene and germanene with non-metallic substrates, Journal of Physics: Conference Series (2015), vol. 574, 012015. DOI:10.1088/1742-6596/574/1/012015
- M. Houssa, E. Scalise, B. van den Broek, A Lu, G Pourtois, V V Afanas'ev and A Stesmans, Interaction of silicene and germanene with non-metallic substrates, ECS Transactions in 2014, DOI: 10.1149/06408.0111ECST
- A. Molle, D. Chiappe, E. Cinquanta, C. Grazianetti, M. Fanciulli, E. Scalise, B. van den Broek, M. Houssa, Structural and chemical stabilization of the epitaxial silicene, ECS Transactions in 2013, DOI: 10.1149/05807.0217ECST

Talk presented at international scientific conferences

- E. Scalise, A. Marzegalli, F. Montalenti, L. Miglio, From the crystal free energy of SiC polytypes to the stacking faults formation energy: a DFT-based lattice-dynamics approach, EMRS Spring Meeting, May 27–31, 2019; Nice, France.
- E. Scalise, A. Marzegalli, F. Montalenti, L. Miglio, Crystal free energy of SiC polytypes and stacking faults formation energy from DFT-based lattice-dynamics approach, APS March Meeting, March 4–8, 2019; Boston, Massachusetts.
- E. Scalise, G. Galli, D. Talapin, S. Wippermann, Characterizing buried nano-interfaces in nanocrystal solids at the atomistic level: a coupled theoretical-experimental approach, APS March Meeting 2018, March 5–9, 2018; Los Angeles, California.
- E. Scalise, M. Houssa, Predicting 2D silicon allotropes on layered chalcogenides, EMRS Spring

Meeting, Strasbourg, France, May 22-26, 2017.

- E. Scalise, S. Wippermann, G. Galli, D. Talapin, Tailoring the electronic properties of semiconducting nanocrystal-solids: InAs embedded in SnSx matrices, DPG-Frühjahrstagung, Dresden, March 19–24, 2017.
- E. Scalise, S. Wippermann, G. Galli, D. Talapin, Tailoring the electronic properties of semiconducting nanocrystal-solids: InAs embedded in SnSx matrices, APS March Meeting 2017, New Orleans, Louisiana, March 13–17, 2017.
- E. Scalise, S. Wippermann, G. Galli, D. Talapin, Probing the interface between semiconducting nanocrystals and molecular metal chalcogenide surface ligands: insights from first principles. APS March Meeting 2016, Baltimore, Maryland, March 14–18, 2016.
- E. Scalise, S. Wippermann, G. Galli, D. Talapin, Probing the interface between semiconducting nanocrystals and molecular metal chalcogenide surface ligands: insights from first principles. 80. Jahrestagung der DPG und DPG-Frühjahrstagung, Regensburg, 6 – 11 March 2016.
- E. Scalise, S. Wippermann, G. Galli, Nanointerfaces in InAs-Sn_2S_6 nanocrystal-ligand networks: atomistic and electronic structure from first principles. 79. Jahrestagung der DPG und DPG-Frühjahrstagung (79th Annual Meeting of the DPG and DPG Spring Meeting), Berlin, 15 - 20 March 2015.
- E. Scalise, S. Wippermann, G. Galli, Nanointerfaces in InAs-Sn_2S_6 nanocrystal-ligand networks: atomistic and electronic structure from first principles. APS March Meeting 2015, San Antonio, Texas, March 2–6, 2015.
- E. Scalise, M. Houssa, B. van den Broek, E. Cinquanta, D. Chiappe, A. Molle, G. Pourtois, V. Afanasiev, A. Stesmans, Theoretical study of 2D silicon nano-lattices, Superstripes Conference, Erice, Italy, July 25-31, 2014. (**Invited**).
- E. Scalise, M. Houssa, B. van den Broek, E. Cinquanta, D. Chiappe, A. Molle, G. Pourtois, V. Afanasiev, A. Stesmans, Theoretical study of silicene on non-metallic substrates with a hexagonal layer structure, EMRS Spring Meeting, Strasbourg, France, May 27-31, 2013.
- E. Scalise, E. Cinquanta, D. Chiappe, C. Grazianetti, B. van den Broek, M. Houssa, M. Fanciulli, A. Molle, Raman spectrum of epitaxial silicene, EMRS Spring Meeting, Strasbourg, France, May 27-31, 2013.
- E. Scalise, M. Houssa, A. Stesmans, P. Geoffrey, V. Afanas'ev. First-principles study of strained 2D MoS_2, EMRS Spring Meeting, Strasbourg, France, May 14-18, 2012.

Poster presented at international scientific conferences

- E. Scalise, F. Grassi, F. Montalenti, L. Miglio. Template effect of the nanowire core on the growth of hexagonal Si/Ge shell: a first principles modeling, Nanowire-week 2019, Pisa, Italy.
- E. Scalise, S. Wippermann, G. Galli, D. Talapin, Tailoring the electronic properties of semiconducting nanocrystal-solids: InAs embedded in SnSx matrices, EMRS Spring Meeting, Strasbourg, France, May 22-26, 2017.
- E. Scalise, S. Wippermann, G. Galli, Nanointerfaces in semiconducting nanocomposites: atomistic and electronic structure from first principles. PSI-K 2015 CONFERENCE, 6-10 September 2015, San Sebastian, Spain.