

EMILIO SCALISE

Surname: Scalise

Name: Emilio

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Telephone: +39-(0)26448-5233

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

Age at graduation: 23

First academic year of enrolment: 2007

Official time limit for the degree course: 2 years

Compulsory thesis: Yes

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

Total number of exams taken abroad that had been
validated: 8

Thesis work carried out abroad: Yes

Compulsory training or internship carried out within the
course of studies :Yes

Place of traineeship/internship: international research
centre

Institution/company/organisation 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,
I-20152 Milan, Italy

02.2014-10.2017 : Post-doc Research fellow.
Max-Planck-Institut für Eisenforschung,
Max-Planck-Straße 1
D-40237 Düsseldorf, Germany

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

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

Technical and management 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, etc.), GW approximation and linear-response techniques.

Expert in modeling and simulation of (quasi) 2D materials

Expert in electrical measurements for nanoelectronic devices

Development and implementation of state-of-the art modeling approaches based on modern physics and chemistry concepts.

Expertise in electronic structure codes (Quantum Espresso, abinit, SIESTA,...)

Knowledge of micro-controllers.

Authors of several publications in international referee journals (see Publication list).

Successfully coordinated Master students projects.

Contributed to several reports and review of the project: "2DNANOLATTICES : A research project funded by the 7th Framework Program of the European Commission –Future and Emerging Technologies (FET)"

Teaching skills

In charge of lectures and exercise sessions of "Fisica II" and "Termodinamica statistica dei Materiali" (2017-2018)

In charge of the laboratorial and exercise sessions in the field of mechanical physics for the undergraduate students (first year) in physics and math. University of Leuven.

Supervisor of Master students of Physics for the Project Work Nanoscience at the University of Leuven

Informatics 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.

List of publications

Scalise Emilio

Degree:

Master in Electronic Engineering, University of Calabria, Italy (2009).

PhD in Science (Physics), Ku Leuven, Belgium (2013)

Articles in internationally reviewed academic journals

Scalise Emilio, Srivastava Vishwas, Janke Eric, Talapin Dmitri, Galli Giulia, Wippermann Stefan. Surface chemistry and buried interfaces in all-inorganic nanocrystalline solids. *NATURE NANOTECHNOLOGY* (2018), vol. 13, p. 841-848, ISSN: 1748-3387, 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 RESEARCH* (2017), p. 1-14, ISSN: 1998-0124, doi: 10.1007/s12274-017-1777-y

E. Scalise and M. Houssa. Predicting 2D silicon allotropes on SnS₂. *NanoResearch* 10, 1697 (2017).

van den Broek, B. ; Houssa, M.; Scalise, E.; Stesmans, A.; Geoffrey, P.; Afanas'ev, V.V. Two-dimensional hexagonal tin: ab initio geometry, stability, electronic structure and functionalization. *2D Mater.* 1, 021004 (2014)

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 MoX₂ and GaX (X = S, Se, Te) chalcogenide templates. *2D Mater.*, 1, 011010 (2014).

Chiappe, D.; Scalise, E.; Cinquanta, E.; Grazianetti, C.; van den Broek, B.; Fanciulli, M.; Houssa, M.; Molle, A. Two-Dimensional Si Nanosheets with Local Hexagonal Structure on a MoS₂ Surface. *Advanced Materials*, 26, 2096-2101 (2014).

Scalise, E.; Cinquanta, E.; Grazianetti, C.; B. Ealet; Houssa, M.; van den Broek, B.; Pourtois, G. Stesmans, A.; Afanas'ev, V.; M. Fanciulli; A. Molle. Vibrational properties of epitaxial silicene layers on (111) Ag. *Applied Surface Science*, 291, 113-117 (2013).

Cinquanta, E.; Scalise, E.; Chiappe, D.; Grazianetti, C.; van den Broek, B.; Houssa, M.; Fanciulli, M.; Molle, A. Getting through the nature of silicene: sp²-sp³ two-dimensional silicon nanosheet, *J. Phys. Chem. C*, 2013, 117 (32), 16719.

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. *Applied Surface Science*, 291, 98-103 (2014).

Houssa, M.; van den Broek, B.; Scalise, E.; Pourtois, G.; Afanas'ev, VV; Stesmans, A. An electric field tunable energy band gap at silicene/(0001) ZnS interfaces. *Phys Chem Chem Phys*. 2013 Mar 21;15(11):3702-5

Scalise, E.; Houssa, M.; Pourtois, G.; van den Broek, B. ; Afanas'ev, V. and Stesmans, A. Vibrational properties of silicene and germanene. *Nano Research*, 6(1),19-28 (2013).

Scalise, E.; Houssa, M.; Stesmans, A.; Geoffrey, P.; Afanas'ev. First-principles study of strained 2D MoS₂. *Physica E*, 56, 416-421(2014).

Scalise, E.; Houssa, M.; Stesmans, A.; Geoffrey, P.; Afanas'ev, V. Strain-induced semiconductor to metal transition in the two-dimensional honeycomb structure of MoS₂. *Nano Research*, 5 (1), 43-48 (2011).

Scalise, E.; Houssa, M.; Pourtois, G.; Stesmans, A.; Afanas'ev, V. Inelastic electron tunneling spectroscopy of HfO₂ gate stacks: a study based on first-principles modeling. *Applied Physics Letters*, 99 (13), 132101 (2011).

Houssa, M.; Scalise, E.; Sankaran, K.; Pourtois, G.; Afanas'ev, V.; Stesmans, A. Electronic properties of hydrogenated silicene and germanene. *Appl. Phys. Lett.* 98, 223107 (2011).

Scalise, E.; Houssa, M.; Pourtois, G.; Afanas'ev, V.; Stesmans, A. Structural and vibrational properties of amorphous GeO₂ from first-principles. *Applied Physics Letters*, 98 (20), 202110-1-202110-3 (2011).

Books

Scalise, E. , "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)

Scalise, E.; Vibrational Properties of Defective Oxides and 2D Nanolattices: Insights from first-principles simulations. *Springer Theses* (2014)

Talk presented at international scientific conferences

Emily V. S. Hofmann, E. Scalise, S. R. Schofield, G. Cappellini, L. Miglio, N.J. Curson, W. M. Klesse, Atomic scale insights on the formation of tin monolayers on germanium, EMRS Fall Meeting 2019, September 16-19 , Warsaw, Poland.

Emilio Scalise, Anna Marzegalli, Francesco Montalenti, Leonida 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.

Emily V. S. Hofmann, E. Scalise, S. R. Schofield, G. Cappellini, L. Miglio, N.J. Curson, W. M. Klesse, Atomic scale insights into Sn on Ge(100): From submonolayers to the formation of Sn wetting layers, 2nd Joint ISTDM / ICSI 2019 Conference, Sunday, June 2nd - Thursday, June 6th, 2019 University of Wisconsin-Madison.

Emilio Scalise, Anna Marzegalli, Francesco Montalenti, Leonida 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.

Emilio Scalise, Giulia Galli, Dmitri Talapin, Stefan 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 SnS_x 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 SnS_x 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-Sn₂S₆ 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-Sn₂S₆ nanocrystal-ligand networks: atomistic and electronic structure from first principles. APS March Meeting 2015, San Antonio, Texas, March 2–6, 2015.

Emilio Scalise, Michel Houssa, Bas van den Broek, Eugenio Cinquanta, Daniele Chiappe, Alessandro Molle, Geoffrey Pourtois, Valery Afanasiev, Andre Stesmans, Theoretical study of 2D silicon nano-lattices, Superstripes Conference, Erice, Italy, July 25-31, 2014.

Houssa, M.; Scalise, E.; van den Broek, B.; Pourtois, G.; Afanas'ev, V.; Stesmans, A., Interaction of Germanene with (0001)ZnSe surface: a theoretical study, ECS Fall Meeting. Boston (USA) October 27- November 1, 2013.

Molle, A.; Chiappe, D.; Cinquanta, E.; Grazianetti, C.; Fanciulli, M., Scalise, E.; van den Broek, B.; Houssa, M., Structural and chemical stabilization of epitaxial silicene, ECS Fall Meeting. Boston (USA) October 27- November 1, 2013.

Emilio Scalise, Michel Houssa, Bas van den Broek, Eugenio Cinquanta, Daniele Chiappe, Alessandro Molle, Geoffrey Pourtois, Valery Afanasiev, Andre Stesmans, Theoretical study of silicene on non-metallic substrates with a hexagonal layer structure, EMRS Spring Meeting, Strasbourg, France, May 27-31, 2013.

Emilio Scalise, Eugenio Cinquanta, Daniele Chiappe, Carlo Grazianetti, Bas van den Broek, Michel Houssa, Marco Fanciulli, Alessandro Molle, Raman spectrum of epitaxial silicene, EMRS Spring Meeting, Strasbourg, France, May 27-31, 2013.

Eugenio Cinquanta, Emilio Scalise, Daniele Chiappe, Carlo Grazianetti, Bas van den Broek, Michel Houssa, Marco Fanciulli, Alessandro Molle, Raman spectrum of epitaxial silicene, MRS Spring Meeting, San Francisco, April 1-5, 2013

Scalise, E., Houssa, M., Stesmans, A., Geoffrey, P., Afanas'ev. First-principles study of strained 2D MoS₂. EMRS Spring Meeting, Strasbourg, France, May 14-18, 2012.

Houssa, M., Pourtois, G., Scalise, E., Afanas'ev, V., Stesmans, A. (2011). Theoretical study of Ge dangling bonds in GeO₂ and correlation with ESR results at Ge/GeO₂ interfaces. ECS Fall Meeting. Boston, USA, 9-14 October 2011. USA: The Electrochemical Society.

Houssa, M., Scalise, E., Sankaran, K., Pourtois, G., Afanas'ev, V., Stesmans, A. (2011). Hydrogenated silicene and germanene: A first-principles study. International Conference on Si epitaxy and Heterostructures. Leuven, Belgium, 28 August-1 September 2011.

Poster presented at international scientific conferences

E. Scalise, S. Wippermann, G. Galli, D. Talapin, Tailoring the electronic properties of semiconducting nanocrystal-solids: InAs embedded in SnS_x matrices, EMRS Spring Meeting, Strasbourg, France, May 22-26, 2017.

Emilio Scalise, Stefan Wippermann, Giulia Galli , Nanointerfaces in semiconducting nanocomposites: atomistic and electronic structure from first principles. PSI-K 2015 CONFERENCE, 6-10 September 2015, San Sebastian, Spain.

Stefan Wippermann, Emilio Scalise, Marton Voros, Adam Gali, Dario Rocca, Gergely Zimanyi, Francois Gygi, Giulia Galli , Semiconducting nanocomposites for use as light absorbers in multi-exciton generation solar cells: insights from ab initio calculations. PSI-K 2015 CONFERENCE, 6-10 September 2015, San Sebastian, Spain.

Awards

Graduate Student Award at EMRS in Strasbourg, Spring meeting 2013, Symposium I: Route to post-Si CMOS devices: from high mobility channels to graphene-like 2D nanosheets.

Nomination as an outstanding Ph.D. thesis by KU Leuven (Belgium) and publication on the “Springer Theses”, special series recognizing outstanding Ph.D. research.

Nanoresearch Top Papers Award 2013 (awarded in 2015)

Nanoresearch Top Papers Award 2012 (awarded in 2015)