



### **Personal data:**

Name: Elena Degoli  
Birth: Modena (Italy), April 12, 1972  
Citizenship: Italian  
Job address: Dept. di Scienze e Metodi dell'Ingegneria,  
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### **Education:**

1986-1991 Scientific diploma at Liceo Scientifico A. Tassoni, Modena.  
Final mark: 60/60.  
1992-1997 Degree in Physics at the University of Modena and Reggio Emilia  
Final mark: summa cum laude.  
Thesis title: Proprietà Ottiche di Strati Ultra Sottili di Silicio.  
1997-2000 Ph.D in Physics at the University of Modena and Reggio Emilia  
Final mark: summa cum laude.  
Thesis title: Si quantum Wells: a Way for Optoelectronics?

### **Advanced Courses and Specialization Schools**

1. Parallel programming school on the Cray T3E system at the CINECA computer center, Bologna, June 16-19, 1997;
2. School of Parallel Programming at the Edinburgh Parallel Computing Center (EPCC) Edinburgh, Scotland, 7 July-15 September 1997;
3. International School of Physics "ENRICO FERMI", Villa Monastero, Varenna, 21-31 July 1998. Topic: Silicon based microphotronics: from basics to applications
4. National School of Physics of Matter, Villa Gualino, Turin, 21 September-2 October 1998.

### **International awards**

- Young Scientist Award of the European Material Research Society E-MRS Spring Meeting, Strasbourg, France, June 16-19, 1998;
- Award for young scientific authors, INFMeeting, Catania, June 14-18, 1999.

### **Stays abroad**

1997: Scholarship at the Edinburgh Parallel Computing Center (Edinburgh, Scotland).  
Project title: "Parallelization Options for the Core Mantle Boundary flow code ITERTRAN".  
Supervisors: Dr. Rob Baxter of the EPCC and Prof. Kathy Whaler, Departement of Geology and Geophysics of the University of Edinburgh.

## **Scholarships**

03/1997-06/1997 INFM contract at the University of Modena (Prof. Olmes Bisi).

07/1997-09/1997 Fellowship at the Edimburgh Parallel Computing Center (Scotland)(Dr. Rob Baxter, EPCC and Prof. Kathy Whaler, Departement of Geology and Geophysics of the University of Edinburgh)

1998: INFM contract at the University of Modena (Prof. Elisa Molinari).

## **Positions:**

2001. INFM contract at the University of Modena (Prof. Stefano Ossicini).

2002-2005 Associate researcher at the University of Modena and Reggio Emilia (Prof. Olmes Bisi).

2006-2015 Assistent professor at the Dept. of Science and Methods of Engineering, University of Modena and Reggio Emilia.

2015-now Associate professor at the Dept. of Science and Methods of Engineering, University of Modena and Reggio Emilia.

## **Qualifications**

October 2004: judged suitable in a competition (CALL INFM 932) for a fixed-term research position.

April 2018: National scientific qualification as full professor for the SSD FIS/03

## **Teaching Activity**

He teaching activity include the courses:

- Mechanics for the Management Engineering degree (from 2020)
- Mechanics for the Engineering for the Smart Industry degree (from 2018)
- Electromagnetism and optics for the Management Engineering degree (from 2016)
- Mechanics and termodinamics for the Management Engineering degree (from 2013 to 2019)
- Modern Physics for the Mechatronic Engineering degree (a.a. 2012-13)
- Materials Physics, for the Mechatronic Engineering degree (from 2006 to 2012)
- Mechanics and termodinamics (exercises course) for the Mechatronic Engineering and Management Engineering degrees (from 1999 to 2005)
- Electromagnetism and optics (exercises course) for the Mechatronic Engineering and Management Engineering degrees (from 1999 to 2005)

For many years she has been a member of the doctoral college in "Nanoscience and Nanotechnology" and in "Physics and Nano Sciences" at the University of Modena and Reggio Emilia.

## **Publishing activity**

2001: Optoelectronic interconnects for integrated circuits Achievements 1998 - 2001 Silicon based interconnects Edited by Elena Degoli. Luxembourg: office for official Publications of the European Communities.

Since 2014 member of the Editorial Review Board of Thin Solid Films (a specialty of Frontiers in Materials).

She is also partner of the Nature Publishing Group

She is editorial reviewer for Physical Review Letters, Europhysics Letters, Physical Review B, Surface Science, Physica E, The Journal of Physical Chemistry Physica Status Solidi, Journal of Nanotechnology, Materials Science and Engineering B and others.

She is also project reviewer for the American National Science Foundation, for the Italian-German University and for the CINECA supercomputing center.

### **Associations**

- an associate member of the Istituto Nazionale per la Fisica della Materia (INFN) from its foundation to its closure.
- an associate member of the National Research Center- CNR-S3 (today, Nanoscience Institute CNR-S3-NANO) (<http://www.nano.cnr.it/?ente=globale>)
- a member of the interdepartmental Center for industrial research and technology transfer En&Tech which is part of the High-Technology Network of Emilia Romagna (<http://www.enotech.unimore.it/site/home.html>)

### **Research interests:**

Her scientific activity is framed in the field of condensed matter physics with particular reference to the use of computational simulation for the study and design of new materials with specific properties of technological interest in the field of nanotechnologies for photovoltaics, electronics, optoelectronics, photonics and for energy storage.

The main topics addressed in the research from 1998 to today have concerned the study, characterization, design and prediction of the structural, electronic, optical (linear and non-linear) and transport properties of solid state systems using first principle methods (all electron methods, pseudopotential approaches, molecular dynamics).

The main research topics are:

- Si and Ge nanostructures (2-, 1-, 0-dimensional) for applications in photonics, photovoltaics and Li-ion batteries.
- Lead chalcogenide nanostructures, mainly PbS and PbSe nanocrystals, of particular interest in the photovoltaic field.
- Non-linear optical properties of Si-based systems as a new frontier for photonics.
- Transport in high-K materials for application in memory devices.
- Multicrystalline materials for applications in photovoltaic and memory devices.

The effects induced by dimensionality, surface passivating agents, impurities, symmetry, strain as well as point and extended defects (grain boundaries) on the materials properties have been studied.

The results of these investigations have been presented in more than 40 international conferences, published in more than 65 papers on peer-reviewed journals, obtaining more than 1600 citations and an H-index=21 (font: ISI Web of Knowledge, January 2021).

The outcomes of her researches has been acknowledged by 2 international young scientist awards

She has worked and works in many national and international projects (EC SBLED, EC SMILE, EC ESPRIT II MELARI, CNR MADESS II, PRIN1999 Modesti, PRIN2002 Ossicini, INFM PRA RAMSES and INFM PAIS CELEX, PRIN2005 Ossicini, PRIN2007 Ossicini, EC STREP 2010 NASCENT Nanostructured Silicon for tandem solar cell, as well as in bilateral projects with France (Galileo) and Germany (CRUI-Vigoni)) and is currently involved in the EU BAT4EVER 2020-2023: Autonomous Polymer based Self-Healing Components for high performant Lithium Ion Batteries (Research and Innovation action, Building a Low-Carbon, Climate Resilient Future: Next-Generation Batteries).

She coordinated an international research project that involved 5 research groups from Italy, France, Spain, Germany and China.

She also has fruitful collaborations with the supercomputing centers CINECA (Bologna) and previously CASPUR (Rome): she has been and is currently responsible for various supercomputing projects for millions of computing hours.

### **Main Publications:**

1) Ab initio study of oxygen segregation in silicon grain boundaries: The role of strain and vacancies

Maji, R.; Luppi, E.; Capron, N.; Degoli, E.  
ACTA MATERIALIA 204, 116477-116487 (2021)

2) The role of Si vacancies in the segregation of O, C, and N at silicon grain boundaries: An ab initio study

Maji, R.; Contreras-Garcia, J.; Capron, N.; Degoli, E.; Luppi, E..  
THE JOURNAL OF CHEMICAL PHYSICS 155:17, 174704-174714 (2021)

3) First Principle Studies of B and P Doped Si Nanocrystals.

Marri, Ivan; Degoli, Elena; Ossicini, Stefano  
PHYSICA STATUS SOLIDI. A, APPLICATIONS AND MATERIALS SCIENCE 215,  
1700414-1 (2018)

4) Doped and codoped silicon nanocrystals: The role of surfaces and interfaces.

Marri, Ivan; Degoli, Elena; Ossicini, Stefano  
PROGRESS IN SURFACE SCIENCE 92, 375 (2017)

5) Determination of the Electronic Energy Levels of Colloidal Nanocrystals using Field-Effect Transistors and Ab-Initio Calculations

Satria Zulkarnaen Bisri, Elena Degoli, Nicola Spallanzani, Gopi Krishnan; Bart Jan Kooi; Corneliu Ghica, Maksym Yarema, Wolfgang Heiss, Olivia Pulci, Stefano Ossicini, Maria Antonietta Loi  
Advanced Materials 26, 5639 (2014).

6) Second-harmonic generation in silicon waveguides strained by silicon nitride

M. Cazzanelli, F. Bianco, E. Borga, G. Pucker, M. Ghulinyan, Elena Degoli, E. Luppi, V. Vénier, S. Ossicini, D. Modotto, S. Wabnitz, R. Pierobon & L. Pavesi  
Nature Materials 11, 148 (2012) .

7) Size, oxidation, and strain in small Si/SiO<sub>2</sub> nanocrystals,

R. Guerra, Elena Degoli, S. Ossicini, Phys. Rev. B 80, 155332 (2009).

8) Silicon nanocrystallites in a SiO<sub>2</sub> matrix: Role of disorder and size, R. Guerra, I. Marri, R. Magri, L. Martin-Samos, O. Pulci, Elena Degoli, S. Ossicini  
Phys. Rev. B 79, 155320 (2009).

9) Optical Absorption Spectra of doped and codoped Si nanocrystallites,  
L. E. Ramos, Elena Degoli, G. Cantele, Stefano Ossicini, D. Ninno, J. Furthmüller, F. Bechstedt,  
Physical Review B 78, 235310(1-11) (2008).

10) Thomas-Fermi model of electronic screening in semiconductor nanocrystals,  
D. Ninno, F. Trani, G. Cantele, K. J. Hameeuw, G. Iadonisi, Elena Degoli and S. Ossicini,  
Europhys. Lett., 74, pp. 519–525 (2006).