Curriculum Vitæ

Davide Donadio

- **Address:**

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- **Profile:**
  - *Technical areas of expertise:* materials science, statistical mechanics, computational chemistry.
  - *Specialized expertise:* Molecular dynamics, electronic structure theory, transport phenomena, phase transitions, high pressure physics, free energy methods, high performance computing.

- **Education:**
  - **Master in Physics** "Laurea in Fisica", *with honors* at the University of Milan in 1998. Supervisor: Prof. G. Benedek. Dissertation: *"Numerical simulation of the growth of carbon films by molecular beam deposition"*
  - **Ph.D. in Materials Science** at the University of Milan in 2003. Supervisors: Prof. G. Benedek and Prof. M. Bernasconi. Dissertation: *"Photosensitivity and photoelasticity of amorphous silica from first principles"*

- **Appointments:**
  - **Since Jul. 2010: Head of a Max Planck Research Group at the Max Planck Institute for Polymer Research, Mainz.**
  - Jan. 2010 - Jun. 2010: Project Leader at the Max Planck Institute for Polymer Research, Mainz.
  - 2008 - 2009 Staff scientist at the University of California Davis (Chemistry).
  - 2007 - 2008 Postdoctoral fellow in the group of Prof. G. Galli, University of California at Davis (Chemistry).
  - 2003 - 2006 Postdoctoral fellow in the group of Prof. M. Parrinello, ETH Zürich, Switzerland.
  - 1998 - 2003 Ph.D. student at the University of Milano Bicocca (interrupted for 1 year for military service).

- **Habilitation:**
  - Habilitation for full professorship awarded by the Italian ministry of science and education in December

2013.

- **Grants and awards:**
  - FP7-ICT European Coordination Action "EUPHONON", starting in November 2013.
  - FP7-ENERGY European collaborative grant "MERGING" 0.4 million euro (total budget 3 M euro). Funding period 3 years, from 01/2013.
  - Max Planck Research Group grant of 1.25 million euro, awarded by the Max Planck Society from 07/2010 to 06/2015 (5 years).
  - NIC-Juelich computing award on IBM BlueGene JUGENE for 20 million CPU hours for 2012 to study heat transport in graphene.
  - Young Scientist Award of the National Institute for the Physics of Matter - INFM (Italy)1998.
- **Teaching:**
  - **General qualifications:** I am qualified to teach fundamental physics courses, chemical physics, solid state physics and surface science at undergraduate level, and more specific courses on statistical thermodynamics and simulation techniques for postgraduates. I can also provide classes for advanced learners about, materials for energy and state-of-the-art simulation methods.
  - **Teaching appointments:**
  - Since 2011 Faculty member of the Max Planck Graduate Center (MPGC).
  - 2011/2012 (Summer semester) - "Ab initio molecular dynamics: basic theory and advanced methods", at Johannes Gutenberg University, Mainz.
  - 2010/2011 (Winter semester) - "Advanced MD simulation techniques", at Max Planck Institute for Polymer Research and Johannes Gutenberg University, Mainz.
  - 2002/2003 - Teaching assistant at the Department of Physics of the Università di Milano Bicocca. "Elementi di Struttura della Materia (Structure of matter)."
  - 2001/2002 - Teaching assistant at the Department of Physics of the Università di Milano Bicocca. "Esercitazioni di Struttura della Materia (Structure of matter), 1 and 2."
  - **Mentoring:** I have supervised the research of the following graduate students: Federica Trudu (ETH Zürich 2003-2006) , Oliviero Andreussi (Scuola Normale Superiore Pisa 2004-2008), Esther Molina-Montes (University of Granada 2004-2008), Cui Zhang (UC Davis 2008-2011), Yuping He (UC Davis, 2008-2011). I am currently mentoring three Ph.D students in Physics at JGU Mainz, and one Ph.D student of the Max Planck Graduate Center.

- **Invited Lectures:**
- *Atomistic simulations of heat transport: methods and applications* , CUSO school on Simulating activated processes in physics and chemistry: theoretical foundations, Villars, Switzerland, 2013.
- *Atomistic simulations of thermal transport in nanostructured semiconductors*, ICTP Advanced Workshop on Energy Transport in Low-D systems, Trieste, Italy, 2012.
- *Multiscale aspects of thermal transport modeling*, lecture at the KITP workshop "Physical Principles of Multiscale Modeling, Analysis and Simulation in Soft Condensed Matter", UCSB, 2012.
- *Topology and phase transitions in ice and water*, 37th Course of the School of Solid State Physics, "Low-dimensional dynamical phenomena and simulations", at the EMCSC, Erice (Italy), 2006.

- **Service:**
- Member of the directorial board of the Max Planck Institute for Polymer Research since 2010.
- Member of the Scientific Advisory Board of the following international conferences: Phononics2013 and 6th Forum on New Materials, CIMTEC 2014.
- Organizer of the Mainz Materials Simulations Days 2013, sponsored by CECAM, Mainz.
- Organizer of a CECAM workshop on Thermal and electronic transport at the nanoscale, Lugano, June 2011.
- Reviewer for national funding and national evaluation agencies: NSF (USA), Swiss National Science Foundation, ANVUR (Italy).
- Reviewer for several peer-reviewed international journals, among which: Phys. Rev. Lett., Appl. Phys. Lett., Phys. Rev. B, J. Chem. Phys., Europhys. Lett., Eur. Phys. J. B, Nano Letters, ACS-Nano and J. Chem. Theo. and Comput.

- **Research activity:**

In the Max Planck Research Group for Nanostructures and transport at MPIP we perform atomistic simulations of materials, and nanostructures, addressing the challenge of bridging the gap between simulations and experiments. My present research activities focus on non-equilibrium processes, which range from the investigation of assembly and crystallization to the characterization of energy transport properties in complex systems, soft matter and interfaces. To this end we carry out an intense activity of methodological development, which summons traditional all-atom molecular dynamics, electronic structure theory, and rare events techniques, towards a comprehensive theoretical approach able to cover several time and length scales. This research philosophy is currently put into effect in the following projects. The common denominator of these projects is the use of molecular modeling techniques and particle-based methods. Interatomic interactions

are treated either by first principle methods or by empirical forcefields, depending of the main focus of the project.

- Thermal transport in nanostructures and thermoelectric materials.
- Polymer assisted crystallization and biomineralization.
- First principles investigation of water and electrolyte solutions.
- Surface and interface chemistry.
- Development of new algorithms and methods for multiscale modeling.

The results of these ongoing investigations and of my past activities have been published in more than 60 articles in peer-reviewed journals, and one book chapter, and have been the subject of about 40 invited lectures or invited talks at international conferences.

- **Invited seminars and invited talks at international conferences:**
  - *Growth and Properties of Cluster Assembled Carbon Films: Molecular Dynamics Simulations*, NANOMAT 2003, Bruxelles (Belgium), 2003.
  - *Exploring free energy surfaces by molecular dynamics*, CECAM Workshop: "Continuing Challenges in Free Energy Calculations", Lyon (France), 2004.
  - *Surface relaxation of amorphous silica*, "Chromium meeting", Torino (Italy), 2004.
  - *Order parameters in melting and crystallization processes*, CECAM Workshop: "Simulation of rare events: the reaction coordinate problem in complex systems", Lyon (France), 2005.
  - *Simulation of nucleation events in first order phase transitions*, Symposium "Computational Chemistry of Molecular Nanostructures", Karlsruhe (Germany), 2006.
  - *Simulation of nucleation events in first order phase transitions*, invited seminar at the Department of Chemistry, UC Davis (USA) 2006.
  - *Simulation of nucleation events in first order phase transitions*, invited seminar at the Max Planck Institute for Polymer Research, Mainz (Germany), 2006.
  - *Nucleation events in liquid-solid phase transitions*, invited seminar at the Department of Materials Science, University of Milano Bicocca, Milano (Italy), 2006.
  - *Thermal conductivity of carbon nanotubes*, invited seminar at RGP, Lugano (Switzerland), 2007.
  - *Heat transport in silicon nanowires by molecular dynamics*, invited talk at the CECAM Workshop "Structural, electronic and transport properties of quantum wires", Lyon (France) 2008.
  - *Surface induced crystallization of tetrahedral liquids*, Euroice 2008 exploratory workshop, Granada, Spain.

- *Atomistic simulations of heat transport in Silicon Nanowires*, Molecular Foundry User Meeting Workshop, at the Lawrence Berkeley National Lab, Berkeley CA, 2008.
- *Thermal transport at the nanoscale*, Total Energy and Force Methods workshop in Trieste, Italy, 2009.
- *Atomistic simulations of heat transport in Silicon Nanowires*, APS March Meeting, Pittsburgh, PA, 2009.
- *Atomistic simulations of heat transport at the nanoscale*, MRS Spring Meeting, San Francisco, CA, 2009.
- *Molecular systems at high pressure*, CECAM Workshop "Structural Transitions in Solids", Lugano (Switzerland) 2009.
- *Thermal transport in silicon nanostructures*, Workshop on high performance ceramics, Hangzhou, China, 2010.
- *Crystal nucleation in tetrahedral liquids*, invited seminar at the SICCAS, Shanghai, China, 2010.
- *Enhanced sampling of nucleation and crystallization phenomena*, SIM2010 workshop, Asia Pacific Center for Theoretical Physics, POSTECH, Pohang, Korea, 2010.
- *Thermal transport in silicon nanostructures*, invited seminar at the ETSC group, Univ. of Pais Bascos, San Sebastian, 2010.
- *Heat transport in nanostructures*, Rhein-Mein Modeling Meeting, Darmstadt, Germany, 2010.
- *Thermal transport in silicon nanostructures*, APS March Meeting, Dallas, 2011.
- *Polymerization of molecular liquids at extreme conditions*, Mainz Materials Simulation Days, Mainz, Germany, 2011.
- *Simulation of phonon transport in real-scale nanowire devices*, NanoWire11 workshop, Plomari Lesvos, Greece, 2011.
- *Thermal transport in thermoelectric materials*, CPMD meeting, Barcelona, Spain, 2011.
- *Heat transport in real scale nano-devices*, SimBioMa, Konstanz, Germany, 2011.
- *Atomistic Simulations of Heat Transport in Nano-materials and Devices*, MRS Spring Meeting, San Francisco, April 2012.
- *Nucleation and Crystal Growth from Atomistic Simulations*, MRS Spring Meeting, San Francisco, April 2012.
- *Nucleation and Crystal Growth from Atomistic Simulations*, Plumed-Meeting, Trieste, Italy, June 2012.
- *Nanoscale heat transport*, invited seminar at the Fritz Haber Institute in Berlin, Germany, June 2012.
- *Atomistic modeling of heat transport: from nanostructured materials to devices*, EMRS fall meeting, Warsaw, Poland, September 2012.

- *Adsorption and chemistry of aromatic molecules and water at stepped metallic surfaces*, invited seminar at the University of Paderborn, Germany, January 2013.
- *Charge and Heat Transport in Low-dimensional Systems*, invited seminar at DIPC, San Sebastian, Spain, January 2013.
- *Thermal transport in low-dimensional nanostructures*, invited seminar at IENS Lille, France, March 2013.
- *Water at interfaces: A multiscale journey*, invited talk at the workshop "Connecting electrochemical and water simulations: Status and future challenges " at Ringberg Castle, Germany, April 2013.
- *Phonon Transport in Graphene: Effects of Strain and of Finite Temperature Gradients*, plenary talk at Phononics2013, Sharm-el-Sheikh, Egypt, June 2013.
- *Thermal conductivity of carbon nanostructures*, invited talk at the TSRC workshop "Thermal transport at the nanoscale", Telluride, US, June 2013.
- *Heat Transport in Carbon Nanostructures from 1D to 3D*, invited talk at the conference Phononics and Thermal Energy Science, PTES2013, Shanghai, PRC, September 2013.
- *Thermal transport in graphene and three-dimensional nanostructured carbon*, keynote talk at TNT2013, Sevilla, Spain, September 2013.
- *Thermal transport in Carbon Nanostructures*, invited talk at the workshop "Hot Nanostructures" at the Lorentz Center, Leiden, The Netherlands, October 2013.
- *Why large scale atomistic simulations are necessary to model thermal transport*, invited seminar at Ecole Centrale Paris, November 2013.
- *Heat transport in nanostructures: discrepancies between equilibrium and non-equilibrium simulations*, at the workshop "Five pieces and a do in computational physics", Rome, Italy, December 2013.

- **International schools:**
  - *Pair correlation in many fermion systems.* EMCSC, Erice (Italy) 1997
  - *Applications of surface sciences techniques.* EMCSC, Erice (Italy) 1998
  - *Defects in SiO_2 and related dielectrics: science and technology.* EMCSC, Erice (Italy) 2000
  - *Nanostructured Carbon for Advanced Applications.* EMCSC, Erice (Italy) 2000
  - Introduction to MPI programming on Parallel Systems. CINECA Casalecchio di Reno (Italy) 2000
  - Introduction to FORTRAN 90. CINECA Casalecchio di Reno (Italy) 2000.
  - *Spring College on Numerical Methods in Electronic Structure Theory.* Abdus Salam International Centre for Theoretical Physics. Trieste (Italy) 2001.

- *Photosensitivity in Optical Waveguides.* POWAG summer school, Saintpetersburg (Russia) 2002.

- **Languages:**
  - Italian (native), English (fluent), Spanish (good), Russian (good), German (basic).

LIST OF PUBLICATIONS

- **Articles in peer-reviewed international journals in chronological order:**

1 **D. Donadio**, L. Colombo, P. Milani and G. Benedek: "*Growth of nanostructured carbon films by cluster assembling*", Phys. Rev. Lett **83**, 776 (1999).

2 M. Bogana, **D. Donadio**, G. Benedek and L. Colombo: "*Simulation of Atomic Force Microscopy of Fractal Nanostructured Carbon Films*", Europhys. Lett. **54**, 72 (2001).

3 S. Iarlori, D. Ceresoli, M. Bernasconi, **D. Donadio**, and M. Parrinello: "*Dehydroxylation and silanization of the surfaces of β-cristobalite silica: an ab-initio simulation*", J. Phys. Chem B **105**, 8007 (2001).

4 **D. Donadio**, M. Bernasconi and M. Boero: "*Ab initio Simulations of Photoinduced Interconversions of Oxygen Deficient Centers in Amorphous Silica*", Phys. Rev. Lett. **87**, 195504 (2001).

5 L. Zoppi, L. Colombo and **D. Donadio**: "*Atomic scale characterization of nanostructured a-C:H films.*", Eur. Phys. J. B, **27**, 335 (2002).

6 A. Podestà, G. Fantoni, P. Milani, M. Ragazzi, **D. Donadio** and L. Colombo "*Nanofriction study of nanostructured carbon films grown by Supersonic Cluster Beam Deposition*", J. Nanosci. Nanotech. **2**, 637 (2002).

7 **D. Donadio**, M. Bernasconi and F. Tassone "*Photoelasticity of crystalline and amorphous silica from first principles*", Phys. Rev. B **68**, 134202 (2003).

8 R. Martonak, **D. Donadio** and M. Parrinello "*Polyamorphism of ice at low temperatures from constant-pressure simulations*", Phys. Rev. Lett. **92**, 225702 (2004).

9 **D. Donadio**, G. Benedek and L. Colombo "*Elastic moduli of nanostructured carbon films*", Phys. Rev. B, **70**, 195419 (2004).

10 **D. Donadio**, M. Bernasconi and F. Tassone "*Photoelasticity of sodium silicate glass from first principles*", Phys. Rev. B **70**, 214205 (2004).

11 **D. Donadio** and M. Bernasconi "*Ab-initio simulation of photoinduced transformation of small rings in amorphous silica*", Phys. Rev. B **71**, 073307 (2005).

12 R. Martonak, **D. Donadio** and M. Parrinello "*Evolution of the structure of amorphous ice - from LDA through HDA to VHDA*", J. Chem. Phys. **122**, 134501 (2005).

13 **D. Donadio**, P. Raiteri and M. Parrinello "*Topological defects and bulk melting of hexagonal ice*", J. Phys. Chem. B **109**, 5421(letter) (2005).

14 O. Andreussi, **D. Donadio**, M. Parrinello and A. Zewail "*Non-equilibrium dynamics and structure of interfacial ice*", Chem. Phys. Lett. **426**, 115 (2006).

15 R. Martonak, **D. Donadio**, A.R. Oganov and M. Parrinello "*Structural transformations in crystalline phases of silica from classical and ab-initio metadynamics*", Nature Materials, **5**, 623 (2006).

16 F. Trudu, **D. Donadio** and M. Parrinello "*Freezing of a Lennard-Jones fluid: From nucleation to spinodal regime*", Phys. Rev. Lett. **97**, 105701 (2006).

17 G. Bussi, **D. Donadio** and M. Parrinello, "*Canonical sampling through stochastic velocity-rescaling*", J. Chem. Phys. **126**, 014101 (2007).

18 R. E. Bulo, **D. Donadio**, A. Laio, F. Molnar, J. Rieger and M. Parrinello, "*Polyacrylate Interaction with Ca2+ Ions in Water; Coiling and Aggregation*", Macromolecules, **40**, 3437 (2007).

19 R. Martonak, **D. Donadio**, A.R. Oganov and M. Parrinello, "*From 4- to 6- coordinated silica: transformation pathways from metadynamics*", Phys. Rev. B, **76**, 014120 (2007).

20 L. delle Site, L. Ghiringhelli, O. Andreussi, **D. Donadio** and M. Parrinello, "*The interplay between surfacewater and hydrogen bonding in a water adlayer on Pt(111) and Ag(111)*", J. Phys.: Condens. Matter, **19**, 242101 (2007).

21 T. Laino, **D. Donadio** and I. W. Kuo, "*Migration of positively charged defects in α-quartz*", Phys. Rev. B **76**, 195210 (2007).

22 F. Bruneval, **D. Donadio** and M. Parrinello "*Molecular dynamics study of the solvation of calcium carbonate in water*", J. Phys. Chem. B **111**, 12219 (2007).

23 **D. Donadio** and G. Galli "*Thermal Conductivity of Isolated and Interacting Carbon Nanotubes: Comparing Results from Molecular Dynamics and the Boltzmann Transport Equation*", Phys. Rev. Lett. **99**, 255502 (2007).

24 F. Zipoli, **D. Donadio** and M. Bernasconi "*Simulation of the grafting of organosilanes at the surface of dry amorphous silica*", J. Phys.: Condens. Matter **20**, 224011 (2008).

25 E. Molina-Montes, **D. Donadio**, A. Hernandez-Laguna, C. I. Sainz-Diaz and M. Parrinello "*DFT Research on the Dehydroxylation Reaction of Pyrophyllite 1. First-Principle Molecular Dynamics Simulations*", J. Phys. Chem. B **112**, 7051 (2008).

26 E. Molina-Montes, **D. Donadio**, A. Hernandez-Laguna and C. I. Sainz-Diaz "*DFT Research on the Dehydroxylation Reaction of Pyrophyllite 2. Characterization of Reactants, Intermediates, And Transition States along the Reaction Path*", J. Phys. Chem. A **112**, 6373 (2008).

27 **D. Donadio**, R. Martonak, P. Raiteri and M. Parrinello "*Effect of temperature and anisotropic pressure on the phase transitions in α-cristobalite.*", Phys. Rev. Lett. **100**, 165502 (2008).

28 J. Behler, R. Martonak, **D. Donadio** and M. Parrinello "*Metadynamics simulation of the high pressure phases of silicon employing a high-dimensional neural network potential*", Phys. Rev. Lett. **100**, 185501 (2008).

29 M. Sharma, **D. Donadio**, E. Schwegler and G. Galli "*IR spectrum of confined water*", Nano Letters, **8**, 2959 (2008).

30 J. Behler, R. Martonak, **D. Donadio** and M. Parrinello "*Pressure-induced phase transitions in silicon studied by neural network-based metadynamics simulations*", Phys. Status Solidi B, **245**, 2618 (2008).

31 **D. Donadio**, G. Cicero, E. Schwegler, M. Sharma and G. Galli "*Vibrational properties of water under confinement: electronic effects.*", J. Phys. Chem. B **113**, 4170 (2009).

32 L. Spanu, **D. Donadio** and G. Galli "*Theoretical investigation of methane under pressure*", J. Chem. Phys. **130**, 164520 (2009).

33 **D. Donadio** and G. Galli "*Atomistic simulations of heat transport in silicon nanowires*", Phys. Rev. Lett. **102**, 195101 (2009).

34 T. Li, **D. Donadio**, L. M. Ghiringhelli and G. Galli "*Surface induced crystallization in supercooled tetrahedral liquids*", Nat. Mater. **8**, 726 (2009).

35 M. Bonomi, D. Branduardi, G. Bussi, C. Camilloni, D. Provasi, P. Raiteri, **D. Donadio**, F. Marinelli, F. Pietrucci, R. A. Broglia, M. Parrinello "*PLUMED: a portable plugin for free-energy calculations with molecular dynamics*", Comp. Phys. Commun. **180**, 1961 (2009).

36 T. Li, **D. Donadio** and G. Galli "*Nucleation of tetrahedral solids: A molecular dynamics study of supercooled liquid silicon*", J. Chem. Phys. **131**, 224519 (2009).

37 F. Gygi, I. Duchemin, **D. Donadio** and G. Galli "*Practical algorithms to facilitate large-scale first-principles molecular dynamics*", J. Phys. Conference Series, **180**, 012074 (2009).

38 **D. Donadio** and G. Galli "*Temperature dependence of the thermal conductivity of thin silicon nanowires*", Nano Lett. **10**, 847 (2010).

39 M. K. Chan, J. Reed, **D. Donadio**, T. Mueller, Y. S. Meng, G. Galli and G. Ceder "*Cluster expansion and optimization of thermal conductivity in SiGe Nanowires.*", Phys. Rev. B **81**, 174303 (2010). Selected as Editors' suggestion.

40 C. Zhang, **D. Donadio** and G. Galli "*First-Principle Analysis of the IR Stretching Band of Liquid Water*", J. Phys. Chem. Lett. **1**, 1398 (2010).

41 E. Molina-Montes, **D. Donadio**, A. Hernandez-Laguna, C. I. Sainz-Diaz "*Exploring the Rehydroxylation Reaction of Pyrophyllite by Ab Initio Molecular Dynamics*", J. Phys. Chem. B **114**, 75937601 (2010).

42 **D. Donadio**, L. Spanu, I. Duchemin, F. Gygi and G. Galli "*Ab initio investigation of the melting line of nitrogen at high pressure*", Phys. Rev. B (Rapid Communication) **82**, 020102 (2010).

43 G. Galli and **D. Donadio** "*Silicon stops heat in its tracks*" Nature Nanotech. **5**, 701 (2010).

44 Y. He, **D. Donadio**, J.-H. Lee, J. C. Grossman and G. Galli "*Thermal Transport in Nanoporous Silicon: Interplay between Disorder at Mesoscopic and Atomic Scales*", ACS-Nano **5**, 1839, (2011).

45 C. Zhang, **D. Donadio**, F. Gygi and G. Galli "*First Principles Simulations of the Infrared Spectrum of Liquid Water using Hybrid Density Functionals*", J. Chem. Theo. Comp. **7**, 1443 (2011).

46 L. Spanu, **D. Donadio**, D. Hohl and G. Galli "*Stability of hydrocarbons in the deep Earth*", Procs. Natl. Acad. Sci. USA, **108**, 6843 (2011).

47 Y. He, **D. Donadio** and G. Galli "*Heat Transport in Amorphous Silicon: Interplay Between Morphology and Disorder*", Appl. Phys. Lett. **98**, 144101 (2011).

48 I. Duchemin and **D. Donadio** "*Atomistic calculation of the thermal conductance of large scale bulk-nanowire junctions* ", Phys. Rev. B **84** 115423 (2011).

49 R. Scipioni, **D. Donadio**, L. M. Ghiringhelli and L. Delle Site "*Proton Wires via One-Dimensional Water Chains Adsorbed on Metallic Steps*" J. Chem. Theo. Comp. **7**, 2681 (2011).

50 Y. He, **D. Donadio** and G. Galli "*Morphology and Temperature Dependence of the Thermal Conductivity of Nanoporous SiGe*" Nano Lett. **11**, 3608 (2011).

51 T. Li, **D. Donadio**, G. Russo and G. Galli "*Homogeneous ice nucleation from supercooled water*", Phys. Chem. Chem. Phys. **13**, 19807 (2011).

52 R. Peköz, X. Feng and **D. Donadio** "*Ab initio characterization of graphene nanoribbons and of their polymer precursors*", J. Phys.: Condens. Matter, **24**, 104023 (2012).

53 I. Duchemin and **D. Donadio** "*Atomistic simulations of heat transport in real-scale silicon nanowire*

devices", Appl. Phys. Lett. **100**, 223107 (2012).

54 G. C. Sosso, **D. Donadio**, S. Caravati, J. Behler and M. Bernasconi, "*Thermal Transport in Phase Change Materials from Atomistic Simulations*", Phys. Rev. B, **86**, 104301 (2012).

55 R. Peköz, K. Johnston and **D. Donadio** "*Adsorption of DCB on Au and Pt stepped surfaces studied using density functional theory with van der Waals interactions*", J. Phys. Chem. C, **116**, 20409 (2012).

56 Y. He, I. Savic, **D. Donadio** and G. Galli "*Lattice Thermal Conductivity of Semiconducting Bulk Materials: Atomistic Simulations*", Phys. Chem. Chem. Phys. **14**, 16209 (2012).

57 **D. Donadio**, L. M. Ghiringhelli and L. Delle Site "*Autocatalytic and Cooperatively Stabilized Dissociation of Water on a Stepped Platinum Surface*", J. Am. Chem. Soc. **134**, 19217 (2012).

58 I. Savic, **D. Donadio**, F. Gygi and G. Galli "*Dimensionality and heat transport in Si-Ge superlattices*", Appl. Phys. Lett. **102**, 073113 (2013).

59 R. Potestio, S. Fritsch, P. Espanol, R. Delgado-Buscaglioni, K. Kremer, R. Everaers, **D. Donadio**, "*Hamiltonian adaptive resolution simulation of molecular liquids*", Phys. Rev. Lett. **110**, 108301 (2013).

60 L.F.C. Pereira and **D. Donadio** "*Divergence of the thermal conductivity in uniaxially strained graphene*", Phys. Rev. B **87**, 125424 (2013), selected as Editors' suggestion.

61 E. Molina-Montes, **D. Donadio**, A. Hernandez-Laguna, M. Parrinello and C. I. Sainz-Diaz "*Water release from pyrophyllite during the dehydroxylation process explored by quantum mechanical simulations.*", J. Phys. Chem. C **117**, 7526 (2013).

62 R. H. Staff, D. Schaeffel, A. Turshatov, **D. Donadio**, H.-J. Butt, K. Landfester, K. Koynov, and D. Crespy, "*Particle Formation in the Emulsion-Solvent Evaporation Process*", Small **9**, 3514, (2013).

63 T. Li, **D. Donadio** and G. Galli, "*Ice nucleation at the nanoscale probes no man′s land of water*", Nature Commun. **4**, 1887 (2013).

64 R. Potestio, P. Espanol, R. Delgado-Buscaglioni, R. Everaers, K. Kremer, **D. Donadio**,"Monte Carlo adaptive resolution simulation of multicomponent molecular liquids", Phys. Rev. Lett. **111**, 061601 (2013).

65 L.F.C. Pereira, I. Savic and **D. Donadio** "*Thermal conductivity of one-, two- and three-dimensional sp^2 carbon*", New J. Phys. **15**, 105019 (2013).

66 S. Fritsch, R. Potestio, **D. Donadio**, K. Kremer, "*Nuclear quantum effects in water: A multi-scale study*", J. Chem. Theo. Comput. (2014) DOI: 10.1021/ct4010504

- **Book chapters:**
  - G. Benedek, M. Bernasconi, **D. Donadio** and L. Colombo: "*Covalent Cluster-Assembled Carbon Solids*" in "Nanostructured Carbon for Advanced Applications", NATO Science series - Kluwer Academic Publishers (2001).