Curriculum vitae of Prof. MARCO BERNASCONI

Present position: Full professor of Theoretical Condensed Matter Physics (PHYS-04/A), Department of Materials Science, University of Milano-Bicocca, since 2016.

Education

- Phd in Theoretical Condensed Matter Physics, SISSA-Trieste (1993), supervisor: Prof. E.Tosatti
- Master in Theoretical Condensed Matter Physics, SISSA-Trieste (1991), supervisor: Prof. E.Tosatti
- Undergraduate degree in Physics, Milano (1988), supervisor: Prof. G. Benedek

Previous positions

- Associate Professor, University of Milano-Bicocca, 2001-2016
- Assistant Professor, University of Milano-Bicocca, 1998-2001
- Assistant Professor, University of Milano, 1996-1998
- Postdoctoral Fellow, Max-Planck-Institut fuer Festkoerperforschung, Stuttgart, 1994-1996
- Postdoctoral Fellow, SISSA-Trieste, 1993-1994

Teaching and supervision

He gave courses on Quantum Mechanics, Introductory Condensed Matter Physics, Condensed Matter Theory for the undergraduate programs in Materials Science and in Physics. Supervision: 24 undergraduate thesis, 13 Phd thesis, 12 postdoctoral fellows.

Research interest

His research activity is dedicated to the development and application of computational modeling to address problems in materials science and condensed matter physics.
He applies methods for electronic structure calculations and molecular dynamics to study materials for applications in microelectronic and photonics. In the last ten years, the research activity has been focused on the ab-initio simulations of materials for phase change non-volatile memories and on the study of the dynamical and chemical reactivity of semiconductor surfaces. In the past, the research activity has also been devoted to the study of phase transitions at high pressures, hydrogen bonded systems, materials for hydrogen storage and solid oxide fuel cells, amorphous oxides for photonics, fullerite and other low Z superconductors.

Publications and invited talks

Over 190 articles on international peer-reviewed journals, two books as editor, 12 invited articles on books, 1 patent. Over 8500 citations and H-index=48 (ISI-Web of Science, January 2025). Over 70 invited talks at international conferences and schools, over 30 invited seminars at Universities, research centers and industries in Italy and abroad.

Funded projects

Local coordinator of European projects Horizon2020 BEFOREHAND (2019-2022), FP7 SYNAPSE (2013-2015), three national project PRIN (2021, 2003, 2001), a regional project funded by Cariplo Foundation (2009-2011). Responsible for the University of Milano-Bicocca of the Spoke 7 of the National Center for HPC, Big Data and Quantum Computing. Responsible of several projects on high performing computing at ISCRA

(Cineca) and Prace (EU-FP7). Research contracts with industries: Pirelli (1998, 2001, 2005), Micron Semiconductors (2014-2023). Responsible for the activity of molecular modeling of the consortium Corimav between Pirelli and the University of Milano-Bicocca (2001-2005). Participation in several other national and regional projects.

Service and other responsibilities

- Dean of the Phd Program in Materials Science and Nanotechnology of the University of Milano-Bicocca (2017-2022).
- Deputy dean of the Phd program in Nanostructures and Nanotechnology of the University of Milano-Bicocca (2008-2010).
- Coordinator of the Commission for High Performance Computing of the University of Milano-Bicocca, 2015-now.
- Coordinator of the research unit of Milano-Bicocca of the Consorzio Nazionale Interuniversitario per le Scienze Fisiche della Materia (CNISM) (2005-2011).
- Member of the Scientific Committee of the Phd program in Materials Engineering of the Politecnico di Milano, 2011-now.
- Member of the Cineca Committee for the acquisition of supercomputers Tier-0 (procurements 2008 e 2015).
- Member of the Scientific Council of the Department of Physical Sciences and Technologies of Matter of the National Research Council (CNR) (2016-now)
- Co-chairman of six international workshop/school. SIF School on *High-Pressure Phenomena*, Varenna (2001); *Low dimensional dynamical phenomena and simulations*, Erice (2007); *Doctorate School in Nanomaterials and Biomaterials*, Rome (2007); *Challenges in the Atomic Scale Modeling of Glasses,* Strasbourg (2012); Symposium *"Non-volatile Memory Devices"* of CIMTEC workshop, Perugia (2016); *7th, 9th, 12th International Workshop on Characterization and Modeling of Memory Devices*, Milano (2016, 2018, 2023).

Publications of Marco Bernasconi

A. Papers on peer-review international journals (Condensed Matter Physics)

2024

190. D. Acharya, O. Abou El Kheir, S. Perego, D. Campi, and M. Bernasconi, *Atomistic Simulations of the Crystallization of Amorphous GeTe Nanoparticles*, **J. Phys. Chem. C** 128, 19380−19391 (2024)

189. S. Xu, D. D. DiJulio, J. I. Marquez Damian, T. Kittelmann, M. Bernasconi, D. Campi, O. Abou El Kheir, S. I. Laporte, B. Rataj, V. Czamler, O. Zimmer, G. Gorini, V. Santoro, and G. Muhre, *Neutron-nucleus and magnetic scattering of paramagnetic oxygen molecule encaged in clathrate hydrate and C_{60}*, **J. Phys: Condens. Matter** 36, 385904 (2024).

188. V. Santoro, O. Abou El Kheir, D. Acharya, M. Akhyani, K.H. Andersen, J. Barrow, P. Bentley, M. Bernasconi, M. Bertelsen, Y. Beßler, A. Bianchi, G. Brooijmans, L. Broussard, T. Brys, M. Busi, D. Campi, A. Chambon, J. Chen, V. Czamler, P. Deen, D. D. DiJulio, E. Dian, L. Draskovits, K. Dunne, M. El Barbari, M. J. Ferreira, P. Fierlinger, V. T. Froest, B.T. Folsom, U. Friman-Gayer, A. Gaye, G. Gorini, A. Gustafsson, C. Happe, M. Hartl, M. Holl, A. Jackson, E. Kemp, Y. Kamyshkov, T. Kittelmann, E.B. Klinkby, R. Kolevatov, S.I. Laporte, B. Lauritzen, W. Lejon, R. Linander, M. Lindroos, M. Marko, J.I. Marquez Damian, T. C. McClanahan, B. Meirose, F. Mezei, K. Michel, D. Milstead, G. Muhrer, A. Nepomuceno, V. Neshvizhevsky, T. Nilsson, U. Odén, T. Plivelic, K. Ramic, B. Rataj, I. Remec, N. Rizzi, E. Rosenthal, L. Rosta, U. Ruecker, S. Samothrakitis, J. R. Selknaes, H. Shuai,S. Silverstein, W.M. Snow, M. Strobl, M. Strothmann, A. Takibayev, R. Wagner, P. Willendrup, S. Xu, S.C. Yiu, L. Yngwe, A.R. Young, M. Wolke, P. Zakalek, L. Zavorka, L. Zanini, and O. Zimmer, *HighNESS Conceptual Design Report: Volume II. The NNBAR Experiments,* **Journal of Neutron Research** 25, 315-406 (2023), published May 2024.

187. V. Santoro, O. Abou El Kheir, D. Acharya, M. Akhyani, K.H. Andersen, J. Barrow, P. Bentley, M. Bernasconi, M. Bertelsen, Y. Beßler, A. Bianchi, G. Brooijmans, L. Broussard, T. Brys, M. Busi, D. Campi, A. Chambon, J. Chen, V. Czamler, P. Deen, D. D. DiJulio, E. Dian, L. Draskovits, K. Dunne, M. El Barbari, M. J. Ferreira, P. Fierlinger, V. T. Froest, B.T. Folsom, U. Friman-Gayer, A. Gaye, G. Gorini, A. Gustafsson, C. Happe, M. Hartl, M. Holl, A. Jackson, E. Kemp, Y. Kamyshkov, T. Kittelmann, E.B. Klinkby, R. Kolevatov, S.I. Laporte, B. Lauritzen, W. Lejon, R. Linander, M. Lindroos, M. Marko, J.I. Marquez Damian, T. C. McClanahan, B. Meirose, F. Mezei, K. Michel, D. Milstead, G. Muhrer, A. Nepomuceno, V. Neshvizhevsky, T. Nilsson, U. Odén, T. Plivelic, K. Ramic, B. Rataj, I. Remec, N. Rizzi, E. Rosenthal, L. Rosta, U. Ruecker, S. Samothrakitis, J. R. Selknaes, H. Shuai,S. Silverstein, W.M. Snow, M. Strobl, M. Strothmann, A. Takibayev, R. Wagner, P. Willendrup, S. Xu, S.C. Yiu, L. Yngwe, A.R. Young, M. Wolke, P. Zakalek, L. Zavorka, L. Zanini, and O. Zimmer, *HighNESS Conceptual Design Report: Volume I,* **Journal of Neutron Research** 25, 85-314 (2023), published May 2024.

186. Yuhan Chen, Davide Campi, Marco Bernasconi, Riccardo Mazzarello, *Atomistic study of the configurational entropy and the fragility of supercooled liquid GeTe,* **Adv. Func. Materials** 34, 2314264 (2024).

185. D. Acharya, O. Abou El Kheir, D. Campi, and M. Bernasconi, *Crystallization kinetics of nanoconfined GeTe slabs in GeTe/$TiTe_2$-like superlattices for phase change memorie*s, **Sci. Rep**. 14, 3224 (2024).

184. O. Abou El Kheir, L. Bonati, M. Parrinello, and M. Bernasconi, *Unraveling the Crystallization Kinetics of the $Ge_2Sb_2Te_5$ Phase Change Compound with a Machine-Learned Interatomic Potential*, **npj Comput. Materials** 10, 33 (2024); https://doi.org/10.1038/s41524-024-01217-6

183. V. Santoro, K. H. Andersen, P. Bentley, M. Bernasconi, M. Bertelsen, Y. Beßler, A. Bianchi, T. Brys, D. Campi, A. Chambon, V. Czamler, D. D. Di Julio, E. Dian, K. Dunne, M. J. Ferreira, P. Fierlinger, U. Friman-Gayer, B. T. Folsom, A. Gaye, G. Gorini, C. Happe, M. Holl, Y. Kamyshkov, T. Kittelmann, E. B. Klinkby, R. Kolevatov, S. I. Laporte, B. Lauritzen, J. I. Marquez Damian, B. Meirose, F. Mezei, D. Milstead, G. Muhrer, V. Neshvizhevsky, B. Rataj, N. Rizzi, L. Rosta, S. Samothrakitis, H. Schober, J. R. Selknaes, S. Silverstein, M. Strobl, M. Strothmann, A. Takibayev, R. Wagner, P. Willendrup, S. Xu, S. C. Yiu, L. Zanini and O. Zimmer, *The HighNESS Project at the European Spallation Source: Current Status and Future Perspectives,* **Nuclear Science and Engineering**, 198, 31-63 (2024), doi.org/10.1080/00295639.2023.2204184.

182. K. Ramić, J. I. Marquez Damian, D. D. Di Julio, T. Kittelmann, D. Campi, M. Bernasconi, A. Gosh, G. Gorini, N. Rizzi, E. Klinkby, V. Santoro, *Advances in Nuclear Data and Software Development for the HighNESS Project*, **Nuclear Science and Engineering** 198, 74-82 (2024); DOI: 10.1080/00295639.2023.2184196

181. S. Cecchi, J. Momand, D. Dragoni, O. Abou El Kheir, F. Fagiani, D. Kriegner, C. Rinaldi, F. Arciprete, V. Holy, B. J. Kooi, M. Bernasconi, and R. Calarco, *Thick does the trick: genesis of ferroelectricity in two-dimensional GeTe-rich $(GeTe)_m(Sb_2Te_3)_n$ lamellae*, **Advanced Science** 11, 2304785 (2024); DOI: 10.1002/advs.202304785.

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180. Shuqi Xu, Sara Isaline Laporte, Douglas D. DiJulio, Jose Ignacio Marquez Damian, Thomas Kittelmann, Marco Bernasconi, Davide Campi, Giuseppe Gorini, and Valentina Santoro, *Theoretical calculations of neutron scattering cross sections for tetrahydrofuran-containing clathrate hydrates at low temperature*, **EPJ Web of Conferences** 286, 06003 (2023).

179. Douglas D. DiJulio, Jose Ignacio Marquez Damian, Marco Bernasconi, Davide Campi, Giuseppe Gorini, Thomas Kittelmann, Esben Klinkby, Gunter Muhrer, Kemal Ramic, Nicola Rizzi, and Valentina Santoro, *Thermal scattering libraries for cold and very-cold neutron reflector materials*, **EPJ Web of Conferences** 284, 17013 (2023).

178. Tomoki Fujita, Yuhan Chen, Yoshio Kono, Seiya Takahashi, Hidetaka Kasai, Davide Campi, Marco Bernasconi, Koji Ohara, Hirokatsu Yumoto, Takahisa Koyama, Hiroshi Yamazaki,Yasunori Senba, Haruhiko Ohashi, Ichiro Inoue, Yujiro Hayashi, Makina Yabashi, Eiji Nishibori, Riccardo Mazzarello, Shuai Wei, *Pressure-induced reversal of Peierls-like distortions elicits the polyamorphic transition in GeTe and GeSe,* **Nat. Commun.** 14, 7851 (2023)

177. S. Perego, D. Dragoni, S. Gabardi, D. Campi, and M. Bernasconi, *Structure and Crystallization Kinetics of as-deposited Films of the GeTe Phase Change Compound from Atomistic Simulations,* **Phys. Status Solidi RRL** *17, 2200433* (2023); https://doi.org/10.1002/pssr.202200433

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176. C. Martella, D. Campi, P. Pani Tummala, E. Kozma, P. Targa, D. Codegoni, M. Bernasconi, A. Lamperti, and A. Molle, *Extreme bendability of atomically thin MoS_2 grown by perylene-based assisted chemical vapor deposition* (2022), **Nanomaterials** 12, 4050 (2022).

175. S. Isceri, D. Dragoni, D. Campi, S. Cecchi and M. Bernasconi. *Geometry of tellurene adsorbed on the Si(111)-($\sqrt{3}\times\sqrt{3}$)R30^o-Sb surface from first principles calculations*, **Physical Chemistry Chemical Physics** 24, 18608 (2022).

174. Daniel T. Yimam, A.J.T. Van Der Ree, Omar Abou El Kheir, Jamo Momand, Majid Ahmadi, George Palasantzas, Marco Bernasconi and Bart J. Kooi, *Phase separation in Ge-rich GST at different length scales: Melt-quenched bulk versus annealed thin films,* **Nanomaterials** 12, 1717 (2022).

173. C. Cheze, F. Righi Riva, G. Di Bella, E. Placidi, S. Prili, M. Bertelli, A. Diaz Fattorini, M. Longo, R. Calarco, M. Bernasconi, O. Abou El Kheir, and F. Arciprete, *Interface formation during the growth of phase change materials heterostructures based on Ge-rich Ge-Sb-Te alloys,* **Nanomaterials** 12, 1007 (2022).

172. D. Baratella, D. Dragoni, and M. Bernasconi, *First principles calculation of transport and thermoelectric coefficients of liquid $Ge_2Sb_2Te_5$*, **Physica Status Solidi RRL** 2100470 (2022); DOI: 10.1002/pssr.202100470.

171. S. Cecchi, I. Lopez Garcia, A. M. Mio, E. Zallo, O. Abou El Kheir, R. Calarco, M. Bernasconi, G. Nicotra, S. M. S. Privitera, *Crystallization and electrical properties of Ge-rich GeSbTe alloy*s, **Nanomaterials** 12, 631 (2022).

170. K. Ramic, T. Kittelmann, D. D. Di Julio, D. Campi, M. Bernasconi, G. Gorini, J. I. Marquez Damian, V. Santoro, *NJOY+NCrystal: an open-source tool for creating thermal neutron scattering libraries with mixed elastic support*, **Nuclear Inst. and Methods in Physics Research A** 1027, 166227 (2022).

2021

169. D. Dragoni, J. Behler, and M. Bernasconi*, Mechanism of amorphous phase stabilization in ultrathin films of monoatomic phase change material*, **Nanoscale** 13, 16146 (2021). DOI:10.1039/d1nr03432d

168. O. Abou El Kheir and M. Bernasconi, *High-throughput calculations on the decomposition reactions of off-stoichiometry GeSbTe alloys for embedded memories*, **Nanomaterials** 21, 2382 (2021).

167. O. Abou El Kheir, D. Dragoni, and M. Bernasconi, *Density functional simulations of decomposition pathways of Ge-rich GeSbTe alloys for phase change memories*, **Phys. Rev. Mater.** 5, 95004 (2021).

166. M. Cobelli, D. Dragoni, S. Caravati, and M. Bernasconi, *Metal-semiconductor transition in the supercooled liquid phase of the $Ge_2Sb_2Te_5$ and GeTe compounds*, **Phys. Rev. Mater.** 5, 045004 (2021).

165. G. Benedek, M. Bernasconi, D. Campi, I. V. Silkin, I. P. Chernov, V. M. Silkin, E. V. Chulkov, P. M. Echenique, J. P. Toennies, G. Anemone, A. Al Taleb, R. Miranda, and D. Farias, *Evidence for a Spin Acoustic Surface Plasmons from Inelastic Atom Scattering*, **Scientific Report** 11, 1506 (2021).

164. E. Zallo, D. Dragoni, Y. Sybina, S. Cecchi, N. I. Borgardt, M. Bernasconi, and R. Calarco, *Evolution of low frequency vibrational modes in ultrathin GeSbTe films*, **Physica Status Solidi RRL** 15, 2000434 (2021). DOI: 10.1002/pssr.202000434

163. D. Baratella, D. Dragoni, D. Ceresoli, and M. Bernasconi, *First Principles Study on the Crystalline $Ga_4Sb_6Te_3$ Phase Change Compound*, **Physica Status Solidi RRL** 15, 2000382 (2021). DOI: 10.1002/pssr.202000382

2020

162. C. Ribaldone, D. Dragoni, and M. Bernasconi, *A first principles study of the switching mechanism in GeTe/InSbTe superlattice*, **Nanoscale Advances** 2, 5209–5218 (2020). DOI: 10.1039/d0na00577k

161. M. Cobelli, M. Galante, S. Gabardi, S. Sanvito, and M. Bernasconi, *A first-principles study of electromigration in the metallic liquid state of GeTe and Sb_2Te_3 phase-change compounds*, **J. Phys. Chem. C** 124, 9599−9603 (2020); DOI:10.1021/acs.jpcc.0c01824

160. A. Ruckhofer, D. Campi, M. Bremholm, P. Hofmann, G. Benedek, M. Bernasconi, W. E. Ernst and A. Tamtögl, *Terahertz Surface Modes and Electron-Phonon Coupling on Bi_2Se_3(111),* **Physical Review Research** 2, 023186 (2020).

159. E. Bosoni, D. Campi, D. Donadio, G. C. Sosso, J. Behler, and M. Bernasconi, *Atomistic Simulations of Thermal Conductivity in GeTe Nanowires,* **J. Phys. D: Applied Physics** 53, 054001 (2020).

2019

158. D. Dragoni and M. Bernasconi, *A first-principles study of structural and electronic properties of the liquid, amorphous and supercooled liquid phases of In_2Te_5*, **J. Chem. Phys.** 151, 134503 (2019).

157. G. C. Sosso and M. Bernasconi, *Harnessing Machine Learning Potentials to Understand the Functional Properties of Phase Change Materials*, **MRS Bulletin** 44, 705 (2019).

156. M. Bernasconi, *Atomistic Simulations of Phase Change Materials for Electronic Memories*, **Int. J. Nanoscience** 18, 1940082 (2019).

155. A. Tamtoegl, P. Kraus, M. Mayrhofer-Reinhartshuber, G. Benedek, M. Bernasconi, D. Dragoni, D. Campi, and W. E. Ernst, *Statics and Dynamics of Multivalley Charge Density Waves in Sb(111)*, **NPJ Quantum Materials** 4, 28 (2019).

154. P. Bartlett, A. I. Berg, M. Bernasconi, S. Brown, G. Burr, C. Foroutan-Nejad, E. Gale, R. Huang, D. Ielmini, G. Kissling,V. Kolosov, M. Kozicki, H. Nakamura, K. Rushchanskii, M. Salinga, A. Shluger, D. Thompson, I. Valov, W. Wang, R. Waser and R. S. Williams, *Phase-change memories (PCM) – Experiments and modelling: general discussion,* **Faraday Discussions** 213, 393 (2019).

153. S. Gabardi, G. C. Sosso, J. Behler, and M. Bernasconi, *Priming effects in the crystallization of the phase change compound GeTe from atomistic simulations*, **Faraday Discussions** 213, 287-310 (2019); DOI: 10.1039/c8fd00101d

152. S. Cecchi, D. Dragoni, D. Kriegner, E. Tisbi, E. Zallo, F. Arciprete, V. Holy, M. Bernasconi, and R. Calarco, *Interplay between structural and thermoelectric properties in epitaxial $Sb_{2+x}Te_3$ alloys*, **Adv. Func. Mat.** 29, 1805184 (2019). DOI: 10.1002/adfm.201805184

2018

151. D. Campi, M. Bernasconi, and G. Benedek, *Ab-initio Calculation of Surface Phonons at the Sb_2Te_3(111) surface*, **Surface Science** 678, 46-51 (2018); https://doi.org/10.1016/j.susc.2018.02.010

2017

150. M. Wiesner, A. Trzaskowska, B. Mroz, S. Charpentier, S. Wang,Y. Song, F. Lombardi, P. Lucignano, G. Benedek, D. Campi, M. Bernasconi, F. Guinea, and A. Tagliacozzo, *The electron-phonon interaction at deep Bi_2Te_3-semiconductor interfaces from Brillouin light scattering,* **Sci. Rep.** 7, 16449 (2017); DOI:10.1038/s41598-017-16313-5.

149. S. Gabardi, E. Baldi, E. Bosoni, D. Campi, S. Caravati, G. C. Sosso, J. Behler, and M. Bernasconi, *Atomistic Simulation of Crystallization Kinetics and Ageing of GeTe Nanowires*, **J. Phys. Chem. C** 121, 23827–23838 (2017). DOI: 0.1021/acs.jpcc.7b09862

148. D. Dragoni, S. Gabardi, and M. Bernasconi, *First principles study of the liquid and amorphous phases of the In_2Te_3 compound*, **Phys. Rev. Mat.** 1, 035603 (2017).

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146. E. Bosoni, G. C. Sosso, and M. Bernasconi, *Grüneisen parameters and thermal conductivity in the phase change compound GeTe*, **J. Comp. Electr.**, 16, 997-1002 (2017). DOI: 10.1007/s10825-017-1040-5.

145. S. Gabardi, D. Campi, and M. Bernasconi*, Ab initio calculation of thermal boundary resistance at the interface of metals with GeTe, In_3SbTe_2 and In_2GeTe_3 phase change compounds***, J. Comp. Electr.** 16, 1003–1010 (2017); DOI 10.1007/s10825-017-1097-1.

144. D. Campi, L. Paulatto, G. Fugallo, F. Mauri, and M. Bernasconi, *First principles calculation of lattice thermal conductivity in crystalline phase change materials: GeTe, Sb_2Te_3 and $Ge_2Sb_2Te_5$*, **Phys. Rev. B** 95, 024311 (2017).

2016

143. R. Wang, D. Campi, M. Bernasconi, J. Momand, B. J. Kooi, A. Verheijen, M. Wuttig, and R. Calarco, *Ordered Peierls distortion prevented at growth onset of GeTe ultra-thin films*, **Sci. Rep.** 6, 32895 (2016).

142. F. Fabbri, E. Rotunno, E. Cinquanta, D. Campi, E. Bonnini, D. Kaplan, L. Lazzarini, M. Bernasconi, C. Ferrari, M. Longo, G. Nicotra, A. Molle, V. Swaminathan and G. Salviati, *Novel near infra-red emission from crystal defects in MoS_2 multi-layer flakes,* **Nature Commun.** 7, 13044 (2016).

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140. S. Gabardi, S. Caravati, J. H. Los, T. D. Kuehne, and M. Bernasconi, *Influence of the exchange and correlation functional on the structure of amorphous InSb and In_3SbTe_2 compounds*, **J. Chem. Phys.** 114, 204508 (2016); http://dx.doi.org/10.1063/1.4950817.

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2015

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B. Invited Articles on Books

12. G. Benedek, M. Bernasconi, J. P. Toennies, M. J. Verstaete, Surface Phonons: Theoretical Methods and Results, **in Springer Handbook in Surface Science, M. Rocca, T. Rahman, L. Vattuone (Eds**.). (2020), pag. 737-782. https://doi.org/10.1007/978-3-030-46906-1_23

11. S. Caravati, G. C. Sosso, and M. Bernasconi, *"Functional Properties of Phase Change Materials from Atomistic Simulations"* in Molecular Dynamics Simulations of Disordered Materials. From Network Glasses to Phase-Change Memory Alloys, Carlo Massobrio, Jincheng Du, Marco Bernasconi, Philip S. Salmon, Editors, Springer Series in Materials Science Volume 215, p. 415-440 (Springer, Berlin 2015). ISBN: 978-3-319-15674-3 (Print) 978-3-319-15675-0.
10. Marzio De Corato, Davide M. Proserpio, Marco Bernasconi, Giorgio Benedek, *"Two C_{28} Clathrates"*, in Diamond and Related Nanostructures, edited by Mircea Vasile Diudea, Csaba Levente Nagy, Springer series on ***Carbon Materials Chemistry and Physics*** **(Springer, Heidelberg Berlin 2013),** Volume 6, pp 75-89; ISBN: 978-94-007-6370-8.

9. Marzio De Corato, Marco Bernasconi, Luca D'Alessio, Ottorino Ori, Mihai V. Putz, Giorgio Benedek, *"Topological Versus Physical and Chemical Properties of Negatively Curved Carbon Surfaces"*, in Topological Modelling of Nanostructures and Extended Systems, edited by Ali Reza Ashrafi, Franco Cataldo, Ali Iranmanesh, Ottorino Ori, Springer series on ***Carbon Materials Chemistry and Physics*** **(Springer, Heidelberg Berlin 2013),** Volume 7, pp 105-136; ISBN: 978-94-007-6412-5.

8. G. Benedek, M. Bernasconi, E. Cinquanta, L. D'Alessio, and M. De Corato, *"The Topological Background of Schwarzite Physics"*, in **Mathematics and Topology of Fullerenes**, edited by Franco Cataldo, Ante Graovac and Ottorino Ori, Springer series on *Carbon Materials Chemistry and Physics* (Springer, Heidelberg Berlin 2012), Chap. 12.

7. X. Blase, G. Benedek and M. Bernasconi, *"Structural, mechanical and superconducting properties of clathrates"* in **Computer-Based Modeling of Novel Carbon Systems and Their Properties: Beyond Nanotubes**", Edited by L. Colombo and A. Fasolino (Springer, NY 2010), Chap.6, ISBN 978-1-4020-9717-1.

6. M. Bernasconi, *Ghiaccio ad alta pressione* in "Accadueo" a cura di Guido Martinotti (Skira Editore, Milano, maggio 2008).

5. G. Benedek and M. Bernasconi, *Fullerenes: topology and structure,* in **Encyclopedia of Nanoscience and Nanotechnology**, J.A. Schwarz, C. Contescu, and K. Putyera, Eds., Marcel Dekker Inc., 2004; G. Benedek and M. Bernasconi, *Fullerenes: Topology and Structure*, in **Dekker Encyclopedia of Nanoscience and Nanotechnology**, 2nd edition: edited by Cristian I. Contescu and Karol Putyera (CRC Press, 2009) Chap. 121, p. 1360-1374

4. G. Benedek, M. Bernasconi, D. Donadio, and L. Colombo, *Covalent cluster-assembled carbon solids*, in **Nanostructured Carbon for Advanced Application**, edited by G. Benedek, P. Milani and V. Ralchenko, (Kluwer Academic Press, 2001), pag. 89.

3. M. Bernasconi*, Ab inito molecular dynamics simulation of amorphous silica surface*, in **Defects in SiO_2 and related dielectrics**, edited by G. Pacchioni, L. Skuja, and D. Griscom (Kluwer Academic Press, 2000).

2. C .Molteni, L.Colombo, L.Miglio, G.Benedek and M.Bernasconi, *Theory of lattice dynamics and Raman spectra of AlGaAs heterostructures*, in **Elementary Excitations in Solids**, edited by J.C.Birman, C.Sebenne and R.F.Wallis , (Elsevier Science Publishers 1992).

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C. Books and Special Issues (Edited)

4. **Special issue of Physical Chemistry Chemical Physics on "**New trends and challenges in surface phenomena, carbon nanostructures and helium droplets – Festschrift for Giorgio Benedek", M. Bernasconi, R. Diaz Muino, P. M. Echenique, J. R. Manson, S. Miret-Artes, J. P. Toennies, Editors, Volume 24, pag. 28085-28642 (2022).

3. **Molecular Dynamics Simulations of Disordered Materials. From Network Glasses to Phase-Change Memory Alloys,** Carlo Massobrio, Jincheng Du, Marco Bernasconi, Philip S. Salmon, Editors, Springer Series in Materials Science Volume 215, 2015 (Springer, Berlin 2015). ISBN: 978-3-319-15674-3 (Print) 978-3-319-15675-0.

2**. High Pressure Phenomena**, R. J. Hemley, G.L. Chiarotti, M. Bernasconi, and L. Ulivi, Editors (Editrice Compositori, Bologna, 2002), Proceeding del corso CXLVII della Scuola "Enrico Fermi", Varenna, luglio 2001.

1. Special issue of the Journal of Physics Condensed Matter on **"Dynamics of Low-Dimensional System"**, M. Bernasconi, S. Miret-Artes, P. Toennies, Editors, Volume 24, Number 10, 14 March 2012.

D. Patent

1. US patent 2020/0335691 A1, **Transition metal doped Germanium-Antimony-Tellurium (GST) memory device components and composition.** Inventors: P. Fantini, M. Bernasconi, S.

Gabardi. Applicant: Micron Technology Inc.. Appl. N. 16/869,499. Filed 7/5/2020. Pub. Date 22/10/2020.