Curriculum dell'attività scientifica e didattica

Prof. MARCO BERNASCONI

Professore Ordinario per il settore FIS03 - Fisica della Materia - Settore Concorsuale 02/B2 - Fisica Teorica della Materia

Dipartimento di Scienza dei Materiali
Università degli Studi di Milano-Bicocca

Posizioni ricoperte

- Professore ordinario di Fisica Teorica della Materia (02/B2, FIS03), Università di Milano-Bicocca, 2016 - presente.
- Professore associato (02/B2, FIS03), Università di Milano-Bicocca, 2001-2016.
- Ricercatore (FIS03), Università di Milano-Bicocca, 1998-2001; Università di Milano, 1996-1998.
- Postdoc, Max-Planck-Institut fuer Festkoerperforschung, Stuttgart (D), 1994-1996.
- Postdoc, SISSA-Trieste, 1993-1994.

Formazione

- Phd in Fisica Teorica della Materia Condensata, SISSA-Trieste (1993); Master in Fisica Teorica della Materia Condensata, SISSA-Trieste (1991); Laurea in Fisica, Università di Milano (1988).

Insegnamento e Supervisione

Titolare di diversi insegnamenti del SSD FIS03: Teoria Quantistica di Atomi e Molecole, Struttura della Materia, Complementi di Struttura della Materia, per i corsi di laurea triennale in Fisica e Scienza dei Materiali, Teoria della Materia Condensata per il corso di laurea magistrale in Fisica dell'Università di Milano-Bicocca, Fisica dei Semiconduttori per il curriculum di Phd in Teoria della Materia Condensata presso la Sissa di Trieste.
Supervisione: 21 tesi di laurea magistrale, specialistica o V.O., 15 tesi triennali, 11 tesi di dottorato di ricerca, 10 postdoc.

Attività di ricerca

Il Prof. Bernasconi svolge attività di ricerca nell'ambito della fisica teorica della materia condensata, studiando in particolare con calcoli di struttura elettronica e simulazioni atomistiche materiali d'interesse per applicazioni in microelettronica, fotonica ed energia. Negli ultimi anni l'attività di ricerca è stata dedicata alle simulazioni atomistiche ab-initio di materiali per memorie non volatili a cambiamento di fase e allo studio delle proprietà dinamiche e della reattività chimica di superfici di semiconduttori. In passato l'attività di ricerca è stata anche rivolta alla simulazione atomistica ab-initio di transizioni di fase sotto pressione, di sistemi a legame idrogeno, di materiali per celle a combustile e per stoccaggio d'idrogeno, di fulleriti ed altri superconduttori a basso Z, di ossidi amorfi per applicazioni in fotonica.

Produzione scientifica: 178 articoli su riviste internazionali ISI con peer-review, 2 libri come editore, 12 articoli su invito su libri, oltre 7500 citazioni e H-index=48 (ISI Web of Science, Maggio 2023), 1 brevetto, oltre 65 comunicazioni su invito a conferenze e scuole internazionali, oltre 30 seminari su invito presso Università, centri di ricerca ed industrie in Italia e all'estero.

Responsabilità di unità di ricerca in progetti nazionali e internazionali: un progetto Horizon2020 (2019-2022), un progetto EU-FP7 (2013-2015), un progetto della Fondazione Cariplo (2010-2012), tre progetti PRIN (2021, 2008, 2003), un progetto di mobilità bilaterale Italia-Ungheria (2012-2014), responsabile per lo Spoke-7 del Centro Nazionale HPC del Pnrr, numerosi progetti di calcolo parallelo ISCRA (Cineca) e Prace (EU-FP7). Partecipazione ad altri progetti nazionali ed europei (PRIN, Cariplo, INFM, Horizon2020).

Responsabilità di contratti per attività di ricerca con industrie: contratti con Pirelli (1998,2001,2005) e Micron Semiconductor (2014-2023), responsabile della linea di ricerca di modellistica molecolare del Consorzio Corimav tra la società Pirelli e l'Università di Milano-Bicocca (2001-2005).

Attività gestionali, organizzative e di servizio

- Coordinatore del Dottorato in Scienza e Nanotecnologia dei Materiali dell'Università di Milano-Bicocca (gennaio 2017- dicembre 2022).
- Vicecoordinatore del Dottorato in Nanostrutture e Nanotecnologie dell'Università di Milano-Bicocca (2008-2010).
- Coordinatore della "Commissione di Ateneo per il Calcolo ad Alte Prestazioni" dell'Università di Milano-Bicocca, 2015-presente.
- Responsabile dell'Unità di Milano-Bicocca e Rappresentante di Ateneo del Consorzio Nazionale Interuniversitario per le Scienze Fisiche della Materia (CNISM) (2005-2011).
- Membro della commissione Cineca per l'acquisizione di macchine di supercalcolo Tier-0 (procurement 2008 e 2015).
- Membro del Comitato di riferimento del dottorato in Ingegneria dei Materiali del Politecnico di Milano 2011-presente.
- Co-chairman di sette workshop/scuole internazionali. Scuola SIF *High-Pressure Phenomena*, Varenna (2001); *Low dimensional dynamical phenomena and simulations*, Erice (2007); *Doctorate School in Nanomaterials and Biomaterials*, Roma (2007); *Challenges in the Atomic Scale Modelling of Glasses, Strasburgo* (2012); Simposio *"Non-volatile Memory Devices"* del congresso CIMTEC, Perugia (2016); *7th, 9th International Workshop on Characterization and Modeling of Memory Devices*, Milano (2016 e 2018).

Publications of Marco Bernasconi

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

2022

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)-(√3× √3)R30º-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).

147. D. Campi, M. Bernasconi G. Benedek, A. P. Graham, and J. P. Toennies, *Surface lattice dynamics and electron-phonon interaction in cesium ultra-thin films*, **Phys. Chem. Chem. Phys.** 19, 16358 (2017).

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).

141. J. L. Battaglia, A. Kusiak, C. Gaborieau, Y. Anguy, H. T. Nguyen, C. Wiemer, M. Longo, D. Campi, M. Bernasconi, and R. Fallica, *$In_3Sb_\alpha Te_\gamma$ thin film structure and thermal conductivity up to 550°C*, **Physica Status Solidi (RRL)** - Rapid Research Letters, 10, 554-548 (2016); 10.1002/pssr.201600109

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.

139. A. Molle, F. Fabbri, D. Campi, A. Lamperti, E. Rotunno, E. Cinquanta, L. Lazzarini, D. Kaplan, V. Swaminathan, M. Bernasconi, M. Longo, and G. Salviati, *Evidence of native Cs impurities and metal-insulator transition in MoS_2 natural crystals*, **Advanced Electronic Materials** 2, 1600091 (2016). DOI: 10.1002/aelm.201600091.

138. A. Stirling, T. Rozgonyi, M. Krack, M. Bernasconi, *Prebiotic NH_3 formation: Insights from simulations*, **Inorganic Chemistry** 56, 1934-1939 (2016); DOI: 10.1021/acs.inorgchem.5b02911.

137. J. H. Los, S. Gabardi, and M. Bernasconi, T. D. Kuehne, *Inverse simulated annealing: improvements and application to the structure determination of amorphous InSb*, **Comp. Mater. Sci.** 117, 7-14 (2016).

136. G. C. Sosso, J. Behler, and M. Bernasconi, *Atomic mobility in the overheated amorphous state of the GeTe compound for phase change memories*, **Phys. Status Solidi A** 213, 329 (2016); doi:10.1002/pssa.201532378.

2015

135. Z. M. Hund, K. J. Nihill, D. Campi, K. T. Wong, N. S. Lewis, M. Bernasconi, G. Benedek, and S. J. Sibener, *The Vibrational Dynamics and Band Structure of Methyl-Terminated Ge(111)*, **J. Chem. Phys.** 143, 124705 (2015).

134. Z. M. Hund, K. J. Nihill, D. Campi, K. T. Wong, N. S. Lewis, M. Bernasconi, G. Benedek, and S. J. Sibener, *Atomic Surface Structure of CH_3-Ge(111) Characterized by Helium Atom Diffraction and Density Functional Theory*, **J. Phys. Chem. B** 119, 18458 (2015).

133. S. Gabardi, S. Caravati, G. C. Sosso, J. Behler, and M. Bernasconi, *Microscopic origin of resistance drift in the amorphous state of the phase change compound GeTe*, **Phys. Rev. B** 92, 054201 (2015).

132. D. Campi, M. Bernasconi, G. Benedek, J. P. Toennies, *The Surface Dynamics of Xe(111): an Ambiguous Nobility*, **J. Phys. Chem. C** 119, 14579–14584 (2015).

131. D. Farias, D. Maccariello, D. Campi, A. Al Taleb, G. Benedek, M. Bernasconi, R. Miranda, *Low-energy excitations of graphene on Ru(0001)*, **Carbon** 93, 1-10 (2015).

130. E. Rotunno, M. Longo, C. Wiemer, R. Fallica, D. Campi, M. Bernasconi, A. R. Lupini, S. J. Pennycook, L. Lazzarini, *A new Ge-doped Sb-Te polymorph*, **Chemistry of Materials** 27, 4368−4373 (2015).

129. A. Bouzid, S. Gabardi, C. Massobrio, M. Boero, and M. Bernasconi, *First principles study of the amorphous $Ga_4Sb_6Te_3$ phase change alloy*, **Phys. Rev. B** 91, 184201 (2015).

128. D. Campi, E. Baldi, G. Graceffa, G. C. Sosso, and M. Benasconi, *Electron-phonon interaction and thermal boundary resistance at interfaces of $Ge_2Sb_2Te_5$ with metals and dielectrics*, **J. Phys.: Condensed Matter** 27, 175009 (2015).

127. G. C. Sosso, M. Salvalaglio, J. Behler, M. Bernasconi, and M. Parrinello, *Heterogeneous crystallization of phase change materials via atomistic simulations,* **J. Phys. Chem. C** 119*,* 6428 (2015).

126. A. Stirling, T. Rozgonyi, M. Krack, and M. Bernasconi, *Pyrite in contact with supercritical water: The desolation of steam*, ***PhysChemChemPhys*** 17, 17375-17379 (2015).

125. D. Campi, D. Donadio, G. C. Sosso, J. Behler, and M. Bernasconi, *Electron-phonon interaction and thermal boundary resistance at the crystal-amorphous interface of the phase change compound GeTe*, **J. Appl. Phys.** 117, 015304 (2015).

124. S. Caravati and M. Bernasconi, *Influence of the exchange and correlation functionals on the structure of amorphous $Ge_2Sb_2Te_5$*, **Physica Status Solidi B** 252, 260 (2015).

2014

123. M. Rizzi, N. Ciocchini, S. Caravati, M. Bernasconi*,* P. Fantini and D. Ielmini, *Statistics of set transition in phase change memory (PCM) arrays*, **Proceedings IEDM14**, pag. 29.6.1 - 29.6.4, ISBN 978-1-4799-8001-7, (2014).

122. G. C. Sosso, J. Colombo, J. Behler, E. Del Gado, and M. Bernasconi, *Dynamical heterogeneities in the supercooled liquid state of the phase change compound GeTe*, **J. Phys. Chem. B** 118, 13621 (2014).

121. R. D. Brown, Z. M. Hund, D. Campi, L. E. O'Leary, N. S. Lewis, M. Bernasconi, G. Benedek, and S. J. Sibener, *The interaction of organic adsorbate vibrations with substrate lattice waves in methyl-Si(111)-(1×1),* **J. Chem. Phys.** 141, 024702 (2014).

120. G. Benedek, M. Bernasconi, K.-P. Bohnen, D. Campi, E. V. Chulkov, P. M. Echenique, R. Heid, I. Yu. Sklyadneva, J. P. Toennies, *Unveiling mode-selected electron-phonon interactions in metal films by helium atom scattering,* **PhysChemChemPhys** 16, 7159-7172 (2014).

2013

119. G. C. Sosso, G. Miceli, S. Caravati, F. Giberti, J. Behler, and M. Bernasconi, *Fast Crystallization of the Phase Change Compound GeTe by Large Scale Molecular Dynamics Simulations*, **J. Phys. Chem. Lett.** 4, 4241 (2013).

118. J. H. Los, T. D. Kuehne, S. Gabardi, and M. Bernasconi, *First principles study of the amorphous In_3SbTe_2 phase change compound*, **Phys Rev. B** 88, 174203 (2013).

117. R. D. Brown, Z. M. Hund, D. Campi, L. E. O'Leary, N. S. Lewis, M. Bernasconi, G. Benedek, and S. J. Sibener, *The Hybridization of Surface Waves with Organic Adlayer Librations: A Helium Atom Scattering and Density Functional Perturbation Theory Study of Methyl-Si(111)*, **Phys. Rev. Lett.** 110, 156102 (2013).

116. J. H. Los, T. D. Kuehne, S. Gabardi, and M. Bernasconi, *First principles simulation of amorphous InSb*, **Phys. Rev. B** 87, 184201 (2013).

115. S. Caravati, G. C. Sosso, M. Bernasconi, and M. Parrinello, *Density functional simulations of hexagonal $Ge_2Sb_2Te_5$ at high pressure*, **Phys. Rev. B** 87, 094117 (2013).

114. A. Tamtögl, P. Kraus, M. Mayrhofer-Reinhartshuber, W. E. Ernst, D. Campi, M. Bernasconi, and G. Benedek, *Surface and Sub-surface Phonons of Bi(111) Measured with Helium Atom Scattering*, **Phys. Rev. B** 87, 035410 (2013).

2012

113. D. Campi, M. Bernasconi, and G. Benedek, *Electronic Properties and Lattice Dynamics of As(111) Surface*, **Phys. Rev. B** 86, 245403 (2012).

112. G. C. Sosso, J. Behler, and M. Bernasconi*, Breakdown of Stokes-Einstein relation in the supercooled liquid state of phase change materials*, **Physica Status Solidi B** 249, 1880 (2012).

111. D. Campi, M. Bernasconi, and G. Benedek, *Phonons and Electron-Phonon Interaction at the Sb(111) surface*, **Phys. Rev. B** 86, 075446 (2012).

110. S. Gabardi, S. Caravati, M. Bernasconi, and M. Parrinello, *Density functional simulations of Sb-rich GeSbTe phase change alloys,* **J. Phys. Cond. Matter** 24, 385803 (2012).

109. D. Mandelli, S. Caravati, and M. Bernasconi, *Density functional study of the TiN/$Ge_2Sb_2Te_5$ interface*, **Physica Status Solidi B** 249, 2140 (2012).

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

107. G. C. Sosso, G. Miceli, S. Caravati, J. Behler, and M. Bernasconi, *A neural-network interatomic potential for the phase change material GeTe*, **Phys. Rev. B** 85, 174103 (2012).

106. G. Miceli, M. Guzzo, C. Cucinotta, and M. Bernasconi, *First principles study of hydrogen desorption from the $NaAlH_4$ surface doped by Ti clusters*, **J. Phys. Chem. C** 116, 4311 (2012).

105. M. Ceriotti, F. Montalenti, and M. Bernasconi, Density functional study of the decomposition pathways of SiH_3 and GeH_3 at the Si(100) and Ge(100) surfaces, **J. Phys. Cond. Matter** 24, 104002 (2012).

2011

104. C.S. Cucinotta, M. Bernasconi, and M. Parrinello, *Hydrogen oxidation reaction at the Ni/YSZ anode of solid oxide fuel cells from first principles,* **Phys. Rev. Lett.** 107, 206103 (2011).

103. G. Miceli and M. Bernasconi, *First principles study of the hydrogenation process of Li_2NH*, **J. Phys. Chem. C** 115, 13496 (2011).

102. S. Caravati, D. Colleoni, R. Mazzarello, T. Kuehne, M. Krack, M. Bernasconi, and M. Parrinello, *First principles study of nitrogen doping in cubic and amorphous $Ge_2Sb_2Te_5$*, **J. Phys. Cond. Matt.** 23, 265801 (2011).

101. V. Sirtori , R. Rognoni, X. Xu, G. Zangari , G. Fratesi, M. I. Trioni, M. Bernasconi, *Unusually Large Magnetic Anisotropy in Electrochemically Deposited Co-Rich Co-Pt Films,* **ACS Applied Materials & Interfaces** 3, 1800 (2011).

100. G. C. Sosso, S. Caravati, R. Mazzarello, and M. Bernasconi, *Raman spectra of crystalline and amorphous $Ge_2Sb_2Te_5$ from first principles*, **Phys. Rev. B** 83, 134201 (2011).
99. E. Spreafico, S. Caravati, and M. Bernasconi, *First principles study of liquid and amorphous $InGeTe_2$*, **Phys. Rev. B** 83, 144205 (2011).
98. G. Miceli, M. Ceriotti, M. Bernasconi and M. Parrinello, *First principles study of the high temperature phase of Li_2NH*, **J. Phys. Chem. C** 115, 7076 (2011).

97. G. Miceli, M. Ceriotti, M. Bernasconi and M. Parrinello, *Static disorder and structural correlations in the low temperature phase of lithium imide*, **Phys. Rev. B** 83, 054119 (2011).

2010

96. M. Ceriotti, G. Miceli, A. Pietropaolo, D. Colognesi, A. Nale, M. Catti, M. Bernasconi, and M. Parrinello, *Nuclear quantum effects in ab initio dynamics: theory and experiments for lithium imide*, **Phys. Rev. B** 82, 174306 (2010).

95. G. Miceli, C. Cucinotta, M. Bernasconi and M. Parrinello*, First principle study of the $LiNH_2/Li_2NH$ transformation*, **J. Phys. Chem C** 114, 15174 (2010).

94. S. Caravati, M. Bernasconi, and M. Parrinello, *First principles study of the optical contrast in phase change materials*, **J. Phys. Condensed Matter** 22, 315801 (2010).

93. G. Benedek, M. Bernasconi, V. Chis, E.V. Chulkov, P. M. Echenique, B. Hellsing, J.P. Toennies, *Theory of surface phonons at metal surfaces: recent advances*, **J. Phys. Condensed Matter** 22, 084020 (2010).

92. R. Mazzarello, S. Caravati, S. Angioletti-Uberti, M. Bernasconi, and M. Parrinello, *Signature of tetrahedral Ge in the Raman spectrum of phase change materials*, **Phys. Rev. Lett.** 104, 085503 (2010).

91. S. Caravati, M. Bernasconi, and M. Parrinello, *First principles study of liquid and amorphous Sb_2Te_3*, **Phys. Rev. B** 81, 014201 (2010).

2009

90. C.S. Cucinotta, G. Miceli, P. Raiteri, M. Krack, T. Kuehne, M. Bernasconi, and M. Parrinello, *Superionic conduction in substoichiometric LiAl alloy: an ab–initio study*, **Phys. Rev. Lett.** 103, 125901 (2009).

89. G.C. Sosso, S. Caravati, C. Gatti, S. Assoni and M. Bernasconi, *Vibrational properties of hexagonal $Ge_2Sb_2Te_5$ from first principles*, **J. Phys. Condensed Matter** 21, 245401 (2009).

88. S. Caravati, M. Bernasconi, T. D. Kühne, M. Krack, and M. Parrinello, *Unravelling the mechanism of pressure induced amorphization of phase change materials*, **Phys Rev. Lett.** 102, 205502 (2009).

87. S. Caravati, M. Bernasconi, T. D. Kühne, M. Krack, and M. Parrinello*, First principles study of crystalline and amorphous $Ge_2Sb_2Te_5$ and the effects of stoichiometric defects,* **J. Phys. Condensed Matter** 21, 255501 (2009); *errata* 21, 499803 (2009); *errata* 22, 399801 (2010).

86. M. Ceriotti, S. Cereda, F. Montalenti, L. Miglio, M. Bernasconi*, Diffusion and decomposition pathways of SiHx species on the Si (100) surface*, **Phys. Rev. B** 79, 165437 (2009).

85. G.C. Sosso, S. Caravati and M. Bernasconi, *Vibrational properties of crystalline Sb_2Te_3 from first principles*, **J. Phys. Condensed Matter** 21, 095410 (2009).

2008

84. V. Chis, B. Hellsing, G. Benedek, M. Bernasconi, E.V. Chulkov, J.P. Toennies, *Large surface charge-density oscillations induced by second-layer surface phonon resonances*, **Phys. Rev. Lett.** 101, 206102 (2008).

83. F. Pietrucci, M. Bernasconi, A. Laio, and M. Parrinello, *Vacancy-vacancy interaction and oxygen diffusion in stabilized cubic zirconia from first principles*, **Phys Rev. B** 78, 094301 (2008).

82. F. Pietrucci, S. Caravati and M. Bernasconi, *TeO_2 glass properties from first principles*, **Phys. Rev. B 78**, 064203 (2008)

81. F. Zipoli, M. Bernasconi, *Ab-initio study of three-dimensional polymers of C_{60}*, **Phys Rev. B 77**, 115432 (2008).

80. F. Zipoli, S. Cereda, M. Ceriotti, M. Bernasconi, L. Miglio, and F. Montalenti, *First principles study of Si/Ge exchanges at the Si(001) surface*, **Appl. Phys. Lett. 92**, 191908 (2008).

79. F. Zipoli, M. Bernasconi, and D. Donadio, *Simulation of the grafting of organosilanes at the surface of dry amorphous silica,* **J. Phys. Condensed Matter 20,** 22401 (2008).

78. S. Cereda, F. Zipoli, M. Bernasconi, L. Miglio, and F. Montalenti, *Thermal-hydrogen promoted selective desorption and enhanced mobility of adsorbed radicals in silicon film growth,* **Phys Rev. Lett.** 100, 046105 (2008).

2007

77. M. Ceriotti and M. Bernasconi, *Diffusion and desorption of SiH_3 on hydrogenated H:Si(100)-2x1 from first principles*, **Phys Rev. B** 76, 245309 (2007).

76. S. Caravati, M. Bernasconi, T.D. Kuehne, M. Krack, and M. Parrinello, *Coexistence of tetrahedral and octahedral-like sites in amorphous phase change materials*, **Appl. Phys. Lett.** 91, 171906 (2007).

75. V. Chis, B. Hellsing, G. Benedek, M. Bernasconi, and J.P. Toennies, *Evidence of longitudinal resonance and optical subsurface phonons in Al(001),* **J. Phys. Condensed Matter** 19, 305011 (2007).

74. S. Cereda, M. Ceriotti, F. Montalenti, M. Bernasconi, and L. Miglio, *Quantitative estimate of H abstraction by thermal SiH_3 on hydrogenated Si(100)(2x1)*, **Phys Rev. B** 75, 235311 (2007).

73. L. D'Alessio, F. Pietrucci, and M. Bernasconi, *First principles study of the vibrational properties of crystalline Li_2TeO_3*, **J. Phys. Chem. Solids** 68, 438-444 (2007).

72. A. Stirling, M. Bernasconi and M. Parrinello, *Defective pyrite (100) surface: an ab initio study*, **Phys Rev. B** 75, 165406 (2007).

2006

71. F. Zipoli, M. Bernasconi, and G. Benedek, *Electron-phonon interaction in halogen-doped carbon clathrates*, **Phys. Rev. B** 74, 205408 (2006).

70. C. Di Valentin. G. Pacchioni, and M. Bernasconi, *Ab-initio molecular dynamics simulation of NO reactivity on CaO(100) surface*, **J. Phys. Chem. B** 110, 8357-8362 (2006).

69. F. Zipoli, T. Laino, A. Laio, M. Bernasconi, and M. Parrinello, *A Quickstep-based QM/MM method for silica*, **J. Chem. Phys**. 124, 154707 (2006).

68. F. Zipoli and M. Bernasconi, *Ab-initio simulation of grafting of phenylacetylene on hydrogenated surfaces of crystalline silicon catalyzed by Lewis-acid*, **J. Phys. Chem B** 110, 23403-23409 (2006).

67. M. Ceriotti, F. Pietrucci, and M. Bernasconi, *Ab-initio study of the vibrational properties of crystalline TeO_2: the α, β, and γ phases*, **Phys. Rev. B** 73, 104304-1/13 (2006).

66. F. Pietrucci, M. Bernasconi, C. Di Valentin, F. Mauri, and C. Pickard, *EPR g tensor of paramagnetic centers in yttria-stabilized cubic zirconia from first-principles*, **Phys. Rev. B** 73, 134112-1/9 (2006).

2005

65. E. Spanò, M. Bernasconi, and E. Kopnin, *Electron-phonon interaction in hole-doped MgB_2C_2*, **Phys. Rev. B** 72, 14530 (2005).

64. F. Zipoli, M. Bernasconi, and A. Laio, *Ab-initio simulation of Lewis-acid catalyzed hydrosilylation of alkynes*, **ChemPhysChem** 6, 1772 (2005).

63. E. Spanò and M. Bernasconi, *Ab-initio study of the structural and vibrational properties of $Mg(AlH_4)_2$*, **Phys. Rev. B** 71, 174301 (2005).

62. R. Martonak, A. Laio, M. Bernasconi, C. Ceriani, P. Raiteri, F. Zipoli and M. Parrinello, *Simulation of structural phase transitions by metadynamics*, **Zeitschrift fuer Kristallographie**, 220, 489-498 (2005).

61. D. Donadio and M. Bernasconi, *Ab-initio simulation of photoinduced transformation of small rings in amorphous silica*, **Phys. Rev. B** 71, 73307 (2005).

2004

60. G. Ballabio, M. Bernasconi, F. Pietrucci, S. Serra, *Ab-initio study of the surfaces of yttrium-stabilized cubic zirconia*, **Phys. Rev. B** 70, 75417 (2004).

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

58. F. Zipoli, M. Bernasconi, R. Martonak, *Constant pressure reactive molecular dynamics simulation of phase transitions under pressure: the graphite to diamond conversion*, **Eur. Phys. J. B** 39, 43 (2004).

57. I. Spagnolatti, A. Mussi, M. Bernasconi, and G. Benedek, *Vibrational properties of C_{20}-based solids*, **Eur. Phys. J. B** 37, 143 (2004).

2003

56. A. Stirling, M. Bernasconi, and M. Parrinello, *Ab-initio simulation of H_2S adsorption on the (100) surface of pyrite*, **J. Chem. Phys**. 119, 4934 (2003)

55. I. Spagnolatti, M. Bernasconi, and G. Benedek, *Electron-phonon interaction in carbon clathrate hex-C_{40}*, **Eur. Phys. J. B** 34, 63-67 (2003).

54. I. Spagnolatti and M. Bernasconi, *Ab-initio calculation of phonon dispersion relations in alpha-Ga*, **Eur. Phys. J. B** 36, 87-90 (2003).

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

52. I. Spagnolatti, M. Bernasconi, and G. Benedek, *Electron-phonon interaction in carbon schwarzites*, **Eur. Phys. J. B**, 32, 181-187 (2003).

51. A. Stirling, M. Bernasconi, and M. Parrinello, *Ab-initio simulation of water interaction with the (100) surface of pyrite*, **J. Chem. Phys**., 118, 8917 (2003).

50. Z. Iqbal, Y. Zhang, H. Grebel, A. Lahamer, G. Benedek, M. Bernasconi, J. Cariboni, I. Spagnolatti, R. Sharma, F. J. Owens, M. E. Kozlov, K. V. Rao, and M. Muhammed, *Evidence for a solid phase of dodecahedral C_{20}*, **Eur. Phys. J. B**, 31, 509-515 (2003)

49. G. Benedek, M. Bernasconi, and A. Gambirasio, *The carbon clathrate hex-C_{16},* **Physica Status Solidi**, 237, 296-300 (2003).

2002

48. I. Spagnolatti, M. Bernasconi, and G. Benedek, *Electron-phonon interaction in the solid form of the smallest fullerene C_{20}*, **Europhys. Lett.** 59, 572 (2002); *erratum*, 60, 329 (2002).

47. P. Masini and M. Bernasconi, *Ab-initio simulation of hydroxylation and dehydroxylation reactions at surfaces: amorphous silica and brucite*, **J. Phys. Condensed Matter** 14, 4133 (2002).

46. A. Cavalleri, K. Sokolowski-Tinten, D. von der Linde, I. Spagnolatti, M. Bernasconi, G. Benedek, A. Podestà and P. Milani, *Observation of Low-Density Liquid Phase of Carbon by Nonthermal Melting of Fullerite*, **Europhys. Lett.** 57, 281 (2002).

2001

45. D. Donadio, M. Bernasconi, and M. Boero, *Ab-initio simulations of photo-induced interconversions of oxygen deficient centers in amorphous silica*, **Phys. Rev. Lett**. 87, 195504 (2001).

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

43. D. D. Klug, R. Rousseau, K. Uehara, M. Bernasconi, Y. Le Page and J. S. Tse, *Ab Initio Molecular Dynamics Study of the Pressure Induced Phase Transformations in Cristobalite*, **Phys. Rev. B** 63, 104106 (2001)

2000

42. R. Rousseau, M. Boero, M. Bernasconi, M. Parrinello and K. Terakura, *Ab-initio simulation of phase transitions and dissociation of H_2S at high pressure*, **Phys. Rev. Lett**. 85, 1254 (2000).

41. A. Gambirasio, M. Bernasconi, G. Benedek, and P. L. Silvestrelli, *Ab-initio simulations of laser-induced transformations in fullerite*, **Phys. Rev. B** 62, 12644 (2000).

40. M. Bernasconi, S. Gaito and G. Benedek, *Clathrates as effective p-type and n-type tetrahedral carbon semiconductors*, **Phys. Rev. B** 61, 12689 (2000).

39. D. Ceresoli, M. Bernasconi, S. Iarlori, M. Parrinello and E. Tosatti, *Two-membered silicon rings on the dehydroxylated surface of silica*, **Phys. Rev. Lett**. 84, 3887 (2000).

38. A. Gambirasio, M. Bernasconi and L. Colombo, *Laser-induced melting of silicon: a tight-binding molecular dynamics simulation*, **Phys. Rev. B** 61, 8233 (2000).

37. C. Parisi, U. Iessi, M. Bernasconi and L. Miglio, *Role of tight-binding parameters in the calculation of transverse effective charges of semiconductors*, **Phys. Rev. B** 61, 4667 (2000).

1999

36. F. Brugè, M. Bernasconi, and M. Parrinello, *Ab-initio simulation of the rotational dynamics of solvated ammonium ion in water*, **J. Amer. Chem. Soc.** 121, 10883 (1999).

35. A. Gambirasio and M. Bernasconi, *Ab-initio study of boron doping in tetrahedral amorphous carbon*, **Phys. Rev. B** 60, 12007 (1999).

34. L. M. Ramaniah, M. Bernasconi, and M. Parrinello, *Ab-initio molecular dynamics simulation of K^+ solvation in water*, **J. Chem. Phys.** 111, 1587 (1999).

33. R. Rousseau, M. Boero, M. Bernasconi, M. Parrinello and K. Terakura, *Static Structure and Dynamical Correlations in High Pressure H_2S*, **Phys. Rev. Lett.** 83, 2218 (1999).

32. C. Cavazzoni, G. L. Chiarotti, S. Scandolo. E. Tosatti, M. Bernasconi and M. Parrinello, *Superionic and metallic states and water and ammonia at giant planets conditions*, **Science** 283, 44 (1999).

31. G. Stapper, M. Bernasconi, N. Nicoloso, and M. Parrinello, *Ab-initio study of structural and electronic properties of yttria-stabilized zirconia*, **Phys. Rev. B** 59, 797 (1999).

30. F. Brugè, M. Bernasconi, and M. Parrinello, *Density-functional study of hydration of ammonium in water clusters*, **J. Chem. Phys.** 110, 4734 (1999).

1998

29. L. M. Ramaniah, M. Bernasconi, and M. Parrinello, *Density-functional study of hydration of sodium in water clusters*, **J. Chem. Phys.** 109, 6839 (1998).

28. M. Bernasconi, P. L. Silvestrelli and M. Parrinello, *Ab-initio infrared study of the hydrogen bond symmetrization in ice*, **Phys. Rev. Lett.** 81, 1235 (1998).

1997

27. J. S.Tse, D. D. Klug, Y. Le Page and M. Bernasconi, *High Pressure 4-coordinated Structure of* SiO_2, **Phys. Rev. B** 56, 10878 (1997).

26. P.L. Silvestrelli, M. Bernasconi, and M. Parrinello*, Ab-initio infrared spectrum of liquid water*, **Chem. Phys. Lett.** 277, 478 (1997).

25. A. Debernardi, M. Bernasconi, M. Cardona, and M. Parrinello, *Infrared absorption in amorphous silicon from ab initio molecular dynamics*, **Appl. Phys. Lett.** 71, 2692 (1997).

24. M. Odelius, M. Bernasconi and M. Parrinello, *Two Dimensional Ice Adsorbed on Mica Surface*, **Phys. Rev. Lett.** 78, 2855 (1997).

23. M. Bernasconi, G.L. Chiarotti, P. Focher, M. Parrinello and E. Tosatti, *Solid-state polymerization of acetylene: ab initio simulation*, **Phys. Rev. Lett.** 78, 2008 (1997).

1996

22. M. Bernasconi, M. Benoit, M. Parrinello, G.L. Chiarotti, P. Focher and E. Tosatti, *Ab-initio simulation of phase transformations under pressure*, **Physica Scripta** T66, 96 (1996).

21. N. A. Marks, D. R. McKenzie, B. A. Pailthorpe, M. Bernasconi and M. Parrinello, *Ab-initio simulations of tetrahedral amorphous carbon*, **Phys. Rev. B** 54, 9703 (1996).

20. M. Benoit, M. Bernasconi, P. Focher, and M. Parrinello, *New High Pressure Phase of Ice*, **Phys. Rev. Lett.** 76, 2934 (1996).

19. M. Bernasconi, M. Parrinello, G. L. Chiarotti, P. Focher, and E. Tosatti, *Anisotropic a-C:H from compression of polyacetylene*, **Phys. Rev. Lett.** 76, 2081 (1996).

18. N.A. Marks, D.R. McKenzie, B.A. Pailthorpe, M. Bernasconi and M. Parrinello, *Microscopic structure of tetrahedral amorphous carbon*, **Phys. Rev. Lett.** 76, 768 (1996).

1995

17. S. Scandolo, M. Bernasconi, G.L. Chiarotti, P. Focher, and E. Tosatti, *Pressure-induced transformation path of graphite to diamond*, **Phys. Rev. Lett.** 74, 4015 (1995).

16. M. Bernasconi, G.L. Chiarotti, P. Focher, S. Scandolo E. Tosatti, and M. Parrinello, *First Principle Constant Pressure Molecular Dynamics*, **J. Phys. and Chem. of Solids** 56, 501 (1995).

15. M. Bernasconi, G.L. Chiarotti and E. Tosatti, *Theory of structural and electronic properties of alpha-Ga(001) and (010) surfaces*, **Phys. Rev. B** 52, 9999 (1995).

14. M. Bernasconi, G.L. Chiarotti and E. Tosatti, *Ab initio calculations of structural and electronic properties of gallium solid state phases*, **Phys. Rev. B** 52, 9988 (1995).

1994

13. P. Focher, G.L. Chiarotti, M. Bernasconi, E. Tosatti and M. Parrinello, *Structural trasformations via first-principles simulation*, **Europhysics Lett.** 26, 345 (1994).

12. M. Bernasconi, G.L. Chiarotti and E. Tosatti, *Solid-State self-wetting phenomena at the (001) surface of semimetallic alpha-Ga*, **Surf. Sci.** 307-309, 936 (1994).

1993

11. M. Bernasconi, G.L. Chiarotti and E. Tosatti, *The (001) surface of alpha-Ga is covered with GaIII*, **Phys. Rev. Lett.** 70, 3295 (1993).

10. M. Bernasconi and E. Tosatti, *Deconstruction, Disordering and Roughening of Metal Surfaces*, **Surf. Sci. Reports.** 17, 363 (1993).

1992

9. C. Molteni, L. Colombo, L. Miglio, G. Benedek and M. Bernasconi, *Disorder configurations from vibrational structure in $Al_xGa_{1-x}As$ systems*, **Philosophical Magazine** 65, 325 (1992).

1991

8. L. Miglio, C. Molteni and M. Bernasconi, *Assessment of compositional disorder in $Al_xGa_{1-x}As$ superlattices from the analysis of Raman spectra*, **Appl. Phys. Lett.** 59, 788 (1991).

7. M. Bernasconi, L. Colombo, L. Miglio and C. Molteni, *Order-disorder interplay in $Al_xGa_{1-x}As$ superlattices: calculation of infrared and Raman spectra*, **Superlattices and Microstructures** 10, 153 (1991).

6. M. Bernasconi, L. Colombo and L. Miglio, *Vibrational properties and infrared spectra of $Al_xGa_{1-x}As$ systems II: order and disorder features in superlattice configuration*, **Physical Review B** 43, 14457 (1991).

5. M. Bernasconi, L. Colombo, L. Miglio and G. Benedek*, Vibrational properties and infrared spectra of $Al_xGa_{1-x}As$ systems I: average t-matrix approximation versus supercell calculation for homogeneous alloys*, **Physical Review B** 43, 14447 (1991).

1990

4. M. Bernasconi, G. Benedek, and L. Miglio, *Phonon dispersion curves and densities of lithium intercalated iron phosporus trisulphide*, **Il Nuovo Cimento D** 12, 1061 (1990).

1989

3. M. Bernasconi, G. Benedek and L. Miglio, *Lattice dynamics of lithium intercalated iron phosphorus trisulphide*, **Materials Science and Engineering B** 3, 167 (1989).

1988

2. M. Bernasconi, G. Benedek and L. Miglio, *Lattice dynamics of lithium intercalated $FePS_3$ compounds*, **Physical Review B** 38, 12100 (1988).

1. M. Bernasconi, G.L. Marra, G. Benedek, L. Miglio, M. Jouanne, C. Julien, M. Scagliotti and M. Balkanski, *Lattice dynamics of layered MPX_3 (M=Mn, Fe, Ni, Zn; X=S, Se) compounds*, **Physical Review B** 38, 12089 (1988).

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).

1. G. Benedek, M.Bernasconi and L.Miglio, *Lattice dynamics of pure and lithium intercalated transition metal phosporus trichalcogenides,* in **Microionics, Integrable Solid State Batteries**, edited by M.Balkaski, North-Holland (Amsterdam 1991).

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.