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 universitario (FIS03), Università di Milano-Bicocca 1998-2001; Università di Milano 1996-1998.
- Postdoc, Max-Planck-Institut fuer Festkoerperforschung, Stuttgart 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, 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 in Fisica e Scienza dei Materiali dell'Università di Milano-Bicocca, Fisica dei Semiconduttori per il curriculum di Phd in Teoria della Materia Condensata presso la Sissa di Trieste.
Supervisione: 13 tesi di laurea di primo livello, 17 tesi di laurea specialistica, magistrale o V.O., 9 tesi di dottorato di ricerca, 8 postdoc (assegnisti universitari e borsisti).

Attività di ricerca

Il Prof. Bernasconi svolge attività di ricerca nell'ambito della fisica teorica della materia condensata, in particolare nel calcolo della struttura elettronica e nelle simulazioni atomistiche di materiali d'interesse per l'energia e per applicazioni in microelettronica e fotonica. Negli ultimi anni l'attività di ricerca è dedicata alle simulazioni atomistiche ab-initio di materiali per memorie non volatili a cambiamento di fase, di ossidi amorfi per applicazioni in fotonica, 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 e altri superconduttori a basso Z.

Produzione scientifica: 158 articoli su riviste internazionali con peer-review, 2 libri come editore, 10 articoli su invito su libri, oltre 5500 citazioni e H-index=40 (ISI-Web of

Knowledge, Luglio 2019), 60 comunicazioni su invito a conferenze e scuole internazionali, 26 seminari su invito presso Università, centri di ricerca ed industrie in Italia e all'estero.

Collaborazioni scientifiche internazionali: collaborazioni in corso con numerose Università e centri di ricerca tra cui Università di Goettingen (D), Paul Drude Institute (Berlino), CNRS (Strasburgo, F), Università di Graz (Austria), Università di Groeningen, Università di Warwick (UK), Trinity College Dublino.

Responsabile di unità di ricerca in progetti nazionali e internazionali: un progetto Horizon2020 (2019-2021), un progetto EU-FP7 (2013-2015), un progetto della Fondazione Cariplo (2010-2012), due progetti PRIN (2008 e 2003), un progetto bilaterale Italia-Ungheria (2012-2014), numerosi progetti di calcolo parallelo ISCRA (Cineca) e Prace (EU-FP7). Partecipazione ad altri progetti nazionali (PRIN, Cariplo, INFM).

Responsabile di contratti per attività di ricerca con industrie: contratti con le società Pirelli (1998, 2001, 2005) e Micron Semiconductors (2014-2019), responsabile della linea di ricerca di modellistica molecolare del Consorzio Corimav tra la società Pirelli e l'Università di Milano-Bicocca (2001-2005).

Attività di valutazione della ricerca: attività di referee per oltre 50 riviste internazionali di Fisica, Chimica e Scienza dei Materiali tra cui Nature Materials, Science, Phys. Rev. Lett., Advanced Materials, Angewandte Chemie. Attività di referee per progetti internazionali e esteri tra cui NSF e DoE (USA), National Science Foundation di Francia, Svizzera, Austria, Romania, Repubblica Ceca e Belgio.

Attività organizzative

- Coordinatore del Dottorato in Scienza e Nanotecnologia dei Materiali (2017-presente) dell'Università di Milano-Bicocca.
- Vicecoordinatore del Dottorato in Nanostrutture e Nanotecnologie (2008-2010) dell'Università di Milano-Bicocca.
- 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.
- Membro del Comitato Scientifico del Dipartimento di Scienze Fisiche e Tecnologie della Materia del CNR, 2016-presente.

- Co-chairman 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); 7^{th} and 9^{th} *International Workshop on Characterization and Modeling of Memory Devices*, Milano (2016, 2018).

Publications of Marco Bernasconi

A. Papers on peer-review international journals

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.**, in press.

157. G. C. Sosso and M. Bernasconi, Harnessing *Machine Learning Potentials to Understand the Functional Properties of Phase Change Materials*, **MRS Bulletin**, in press.

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

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);

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);

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,
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. Elect.**, 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).

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).

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, *$In_3Sb_bTe_g$ 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.

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 Diffration 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).

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).

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).

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).

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).

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).

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).

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).

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B. Invited Articles on Books

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C. Books and Special Issues (Edited)

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