Curriculum vitae of Prof. MARCO BERNASCONI

Present position: Full professor of Theoretical Condensed Matter Physics (02/B2, FIS/03), Department of Materials Science, University of Milano-Bicocca.

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

- Full Professor, University of Milano-Bicocca, 2016-now
- 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: 20 undergraduate thesis, 10 Phd thesis, 8 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

166 articles on international peer-reviewed journals, two books as editor, 12 invited articles on books, Over 6500 citations and H-index=43 (ISI-Web of Science, April 2021).
Over 60 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 (2019-2021), FP7 SYNAPSE (2013-2015), a national project PRIN2008, a regional project form Cariplo Foundation (2009-2011). 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 (2014-2021). 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-now).
- 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 and 9th International Workshop on Characterization and Modeling of Memory Devices*, Milano (2016, 2018).

Present international scientific collaborations

Collaborations ongoing with several universities and research centers abroad including University of Goettingen (D), Paul Drude Institute (Berlin), University of Bordeaux (F), University of Graz (Austria), University of Warwick (UK), Trinity College Dublin.

Scientific reviewing

Referee activity for over 50 journals on Physics, Chemistry and Materials Science including Nature Materials, Nature Comm., Science, Phys. Rev. Lett., Advanced Materials, Angewandte Chemie. Referee activity for international projects and institutions abroad including ERC, NSF and DoE (USA), National Science Foundations of Switzerland, France, Austria, Romania, and Belgium.

Publications of Marco Bernasconi

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

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.** (2021), in press.

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).

2020

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 (2020). 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 (2020). DOI: 10.1002/pssr.202000382

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. 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); 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).

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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).

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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).

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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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D. Patent

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