

## **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, 14 Phd thesis, 12 postdoctoral fellows.

### **Research interest**

His research activity is dedicated to the development and application of atomistic simulations to address problems in materials science and condensed matter physics. He applies methods for electronic structure calculations, molecular dynamics and machine learning techniques to study materials for applications in microelectronic and photonics. In the last 15 years, the research activity has been mostly focused on the atomistic simulations of materials for phase change non-volatile electronic memories and neuromorphic devices. In the past, the research activity was also devoted to the study of dynamical properties and chemical reactivity of semiconductor surfaces, 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 200 articles on international peer-reviewed journals, two books as editor, 12 invited articles on books, 1 patent. Over 9200 citations and H-index=51 (Scopus, May 2026). Over 70 invited talks at international conferences and schools, over 30 invited seminars at Universities, research centers and industries.

### **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 EuroHPC. Research contracts with industries: Pirelli (1998, 2001, 2005), Micron Semiconductors (8 contracts in 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 European, 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 eight 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); *7<sup>th</sup>, 9<sup>th</sup>, 12<sup>th</sup>, 14<sup>th</sup> International Workshop on Characterization and Modeling of Memory Devices*, Milano (2016, 2018, 2023, 2025).

# Publications of Marco Bernasconi

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

### 2026

201. Omar Abou El Kheir and Marco Bernasconi, *On the origin of in-gap states in amorphous  $Ge_2Sb_2Te_5$* , **Acta Materialia** 312, 122251 (2026).

200. Flavio Giuliani, Francesco Guidarelli Mattioli, Yuhan Chen, Dario Baratella, Daniele Dragoni, Marco Bernasconi, John Russo, Lilia Boeri, and Riccardo Mazzarello, *Liquid Anomalies and Fragility of Supercooled Antimony*, **Proc. Nat. Acad. Sci.** 123, e2531605123 (2026).

199. P. Fantini, A. Ghetti, E. Varesi, A. Pirovano, F. Pellizzer, D. Baratella, C. Ribaldone, S. Caravati, D. Campi, M. Bernasconi, and R. Bez, *Microscopic model of the operation of the Single-chalcogenide X-point Memory*, **Commun. Mater.** 7, 26 (2026).

### 2025

198. Sebastiano Caravati, Dario Baratella, Paolo Fantini, Marco Bernasconi, *In-gap electronic states of  $GeAsSe$  and  $SiGeAsSe$  alloys for selector devices from atomistic simulations*, **Solid State Sciences** 170, 108127 (2025); <https://doi.org/10.1016/j.solidstatesciences.2025.108127>.

197. F. Righi Riva, S. Cecchi, S. Prili, O. Abou El Kheir, E. Placidi, A. Diaz Fattorini, S. Calvi, M. Longo, M. Bernasconi, R. Calarco, and F. Arciprete, *Electronic properties and stacking ordering in layered  $GeTe$ -rich  $(GeTe)_m(Sb_2Te_3)_n$* , **ACS Appl. Electron. Mater.** 7, 9320–9328 (2025).

196. S. Marcorini, R. Pomodoro, O. Abou El Kheir, and M. Bernasconi, *Viscosity, the breakdown of Stokes-Einstein relation and dynamical heterogeneity in supercooled liquid  $Ge_2Sb_2Te_5$  from simulations with a neural network interatomic potential*, **J. Chem. Phys.** 163, 154501 (2025).

195. Matteo Cobelli, Dario Baratella, Paolo Fantini, and Marco Bernasconi, *Ab-initio study of electromigration in liquid  $GeAsSe$  alloys for selector devices*, **J. Chem. Phys.** 163, 084711 (2025); DOI: 10.1063/5.0280879.

194. D. Acharya, O. Abou El Kheir, S. Marcorini, and M. Bernasconi, *Simulation of the crystallization process of  $Ge_2Sb_2Te_5$  nanoconfined in superlattice geometries for phase change memories*, **Nanoscale** 17, 13828-13841 (2025). DOI: 10.1039/d5nr00283d

193. O. Abou El Kheir and M. Bernasconi, *Million-atom simulation of the set process in phase change memories at the real device scale*, **Advanced Electronic Materials** 11, e2500110 (2025); DOI: 10.1002/aelm.202500110

192. S. Ritarossi, R. Piombo, F. Giuliani, D. Dragoni, M. Bernasconi, R. Mazzarello, *Phase-change heterostructures based on antimony*, **Phys. Status Solidi RRL** 2500012 (2025).

191. D. Baratella, O. Abou El Kheir, and M. Bernasconi, *Crystallization kinetics in Ge-rich  $Ge_xTe$  alloys from large scale simulations with a machine-learned interatomic potential*, **Acta Materialia** 284, 120608 (2025).

## 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. Czamlar, 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. Czamlar, 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. Czamlar, 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<sub>2</sub>-like superlattices for phase change memories*, **Sci. Rep.** 14, 3224 (2024).

184. O. Abou El Kheir, L. Bonati, M. Parrinello, and M. Bernasconi, *Unraveling the Crystallization Kinetics of the Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> 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. Czamlar, 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. Kamyshev, T. Kittelmann, E. B. Klinkby, R. Kolevatorov, 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](https://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](https://doi.org/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)<sub>m</sub>(Sb<sub>2</sub>Te<sub>3</sub>)<sub>n</sub> lamellae*, **Advanced Science** 11, 2304785 (2024); DOI: [10.1002/advs.202304785](https://doi.org/10.1002/advs.202304785).

## 2023

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>.

## 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<sub>2</sub> 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)R30°-Sb surface from first principles calculations*, **Physical Chemistry Chemical Physics** 24, 18608 (2022).
174. D. T. Yimam, A.J.T. Van Der Ree, O. Abou El Kheir, J. Momand, M. Ahmadi, G. Palasantzas, M. Bernasconi, and B. 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<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub>*, **Physica Status Solidi RRL** 16, 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, and S. M. S. Privitera, *Crystallization and electrical properties of Ge-rich GeSbTe alloys*, **Nanomaterials** 12, 631 (2022).
170. K. Ramic, T. Kittelmann, D. D. Di Julio, D. Campi, M. Bernasconi, G. Gorini, J. I. Marquez Damian, and 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** 11, 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. Tamtögl, 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

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## 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.