

# Claudio Attaccalite

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PhD

## 12 Selected Publications

1. **Exciton interference in hexagonal boron nitride**  
L. Sponza, H. Amara, F. Ducastelle, A. Loiseau, C. Attaccalite  
Physical Review B **97** (7), 075121 (2018)
2. **Second Harmonic Generation in h-BN and MoS<sub>2</sub> monolayers: the role of electron-hole interaction**  
M. Grüning, C. Attaccalite  
Physical Review B Rapid. Comm. **89**, 081102(R) (2014)
3. **Nonlinear optics from ab-initio by means of the dynamical Berry-phase**  
C. Attaccalite, M. Grüning  
Physical Review B **88** (23), 235113 (2013)
4. **Efficient Gate-tunable light-emitting device made of defective boron nitride nanotubes: from ultraviolet to the visible**  
C. Attaccalite, L. Wirtz, A. Marini, A. Rubio  
Nature Scientific Reports **3**, Article number: 2698 (2013)
5. **First-principles GW calculations for fullerenes, porphyrins, phtalocyanine, and other molecules of interest for organic photovoltaic applications**  
Xavier Blase, Claudio Attaccalite, Valerio Olevano  
Phys. Rev. B **83**, 115103 (2011)
6. **Strong charge-transfer excitonic effects and Bose-Einstein exciton-condensate in graphene**  
Pierluigi Cudazzo, Claudio Attaccalite, Ilya V. Tokatly, Angel Rubio  
Phys. Rev. Lett. **104**, 226804 (2010)
7. **Doped Graphene as Tunable Electron-Phonon Coupling Material**  
C. Attaccalite, M. Lazzeri, L. Wirtz, A. Rubio and F. Mauri  
Nano Letters, **10**(2) 1172 (2010)
8. **Impact of the electron-electron correlation on phonon dispersions: failure of LDA and GGA functionals in graphene and graphite**  
M. Lazzeri, C. Attaccalite, L. Wirtz and F. Mauri  
Phys. Rev. B Rapid Comm. **78**, 081406(R) (2008).
9. **Electron-Electron Correlation in Graphite: A Combined Angle-Resolved Photoemission and First-Principles Study**

- A. Grünis, C. Attaccalite et al.  
Phys. Rev. Lett. **100**, 037601 (2008)
10. **Stable liquid Hydrogen at high pressure by a novel *ab-initio* molecular dynamics**  
C. Attaccalite and S. Sorella  
Phys. Rev. Lett. **100**, 114501 (2008)
11. **Correlated geminal wave function for molecules: an efficient resonating valence bond approach**  
M. Casula, C. Attaccalite, S. Sorella  
Journal of Chem. Phys. **121**, 7110 (2004)
12. **Correlation Energy and Spin Polarization in the 2D Electron Gas**  
C. Attaccalite, P. Gori Giorgi, S. Moroni, G. B. Bachelet  
Phys. Rev. Lett. **88**, 256601 (2002)

■■■■■■■ PhD thesis

1. **RVB phase of hydrogen at high pressure: towards the first *ab-initio* Molecular Dynamics by Quantum Monte Carlo**  
International School for Advanced Studies (SISSA/ISAS), Trieste (Italy)  
Supervisor: Sandro Sorella

Data: 26/04/2018

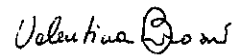
Clouster Attaccalite

MA FJ

### Pubblicazioni allegate

1. *Quantum Interference Assisted Spin Filtering in Graphene Nanoflakes* A. Valli, A. Amaricci, V. Brosco, and M. Capone Nano Letters **18** 2158 (2018)
2. *Pauli metallic ground state in Hubbard clusters with Rashba spin-orbit coupling* Valentina Brosco, Daniele Guerzi, and Massimo Capone Phys. Rev. B **97**, 125103 (2018).
3. *Strong parameter renormalization from optimum lattice model orbitals* V. Brosco, Z.-J. Ying, and J. Lorenzana Phys. Rev. B **95**, 035121 (2017).
4. *Anisotropic transport in Rashba metals* V. Brosco and C. Grimaldi, Phys. Rev. B **95** 195164 (2017).
5. *Unconventional dc Transport in Rashba Electron Gases*, V. Brosco, L. Benfatto, E. Cappelluti, C. Grimaldi, Phys. Rev. Lett. **116** 166602 (2016).
6. *Anomalous scaling and breakdown of conventional density functional theory methods for the description of Mott phenomena and stretched bonds* Z.-J. Ying, V. Brosco, G. Lopez, D. Varsano, P. Gori-Giorgi, and J. Lorenzana Phys. Rev. B **94**, 075154 (2016)
7. *Exact exchange-correlation potential of a Ionic/Mott insulator with a free surface*, V. Brosco, Z. Ying and J. Lorenzana, Nature Scientific Reports **3** , 2172 (2013).
8. *Floquet theory of Cooper pair pumping* A. Russomanno, S. Pugnetti, V. Brosco and R. Fazio, Physical Review B **83** 214508 (2011).
9. *Decoherence in adiabatic quantum evolution-application to Cooper pair pumping*, J. Pekola, V. Brosco, M. Möttönen, P. Solinas, A. Shnirman, Physical Review Letters **105**, 030401 (2010).
10. *Prediction of resonant all electric spin pumping*, V. Brosco, M. Jerger, P. San-José, G. Zarand, A. Shnirman, and G. Schön, Physical Review B (Rapid Communications) **82**, 041309 (2010).
11. *Single qubit lasing in the strong coupling regime*, S. André, P- Q. Jin, V. Brosco, J. H. Cole, A. Romito, A. Shnirman, and G. Schön, Phys. Rev. A **82**, 053802 (2010), selected by S. Girvin for the “cond-mat Journal Club” of September 2010, <http://www.condmatjournalclub.org/?p=1122>.
12. *Non-abelian superconducting pumps*, V. Brosco, R. Fazio, F. W. J. Hekking, and A. Joye, Phys. Rev. Lett. **100**, 027002 (2008).

Rome, 3 Maggio 2018

  
(Valentina Brosco)

## Barbara Capone - 12 Selected Publications and PhD Thesis

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1. E. Bianchi, B. Capone, I. Coluzza, L. Rovigatti, P. J. van Oostrum "Limiting the valence: advances and new perspectives on patchy colloids, soft functionalized nanoparticles and biomolecules", **Physical Chemistry Chemical Physics**, 2017, 19, 19847 - 19868 This article is part of the themed collection: 2017 PCCP HOT Articles
2. E. Locatelli, B. Capone, C. N. Likos "Multiblob coarse-graining for mixtures of long polymers and soft colloids", **J. Chem. Phys.** 145, 17, 174901 (2016)
3. L. Rovigatti, B. Capone, C. N. Likos "Soft self-assembled nanoparticles with temperature dependent properties", **Nanoscale**, 8, 3288 (2016) (This paper makes the second cover page of the Nanoscale Issue)
4. A. Nikoubashman, N. A. Mahynski, B. Capone, A. Z. Panagiotopoulos, and C. N. Likos, Coarse-graining and phase behavior of model star polymer-colloid mixtures in solvents of varying quality, **J. Chem. Phys.**, 143, 243108 (2015)
5. T. A. Grünewald, A. Lassenberger, R. Zirbs, B. Capone, P. van Oostrum, I. Vonderhaid, H. Lichtenegger, and E. Reimhult "Core-shell structure of monodisperse PEG-coated iron oxide nanoparticles for biomedical applications", **Chem. Mater.**, 27 (13), 4763 (2015)
6. E. Bianchi, B. Capone, G. Kahl and C. N. Likos "Soft-patchy nanoparticles: modeling and self-organization", **Faraday Discuss.**, 181, 123-138 (2015)
7. A. Narros, C. N. Likos, A. Moreno, B. Capone "Multi-blob coarse graining for ring polymer solutions", **Soft Matter**, 10, 9601 (2014) (This paper makes the cover page of the Soft Matter Issue)
8. D. Truzzolillo, D. Marzi, J. Marakis, B. Capone, M. Camargo, A. Munam, M. Gauthier, C. N. Likos, D. Vlassopoulos "Glassy states in asymmetric mixtures of soft and hard colloids", **Phys. Rev. Lett.**, 111, 208301 (2013)
9. I. Coluzza, P. van Oostrum, B. Capone, E. Reimhult, C. Dellago, "Folding and design of self-knotting colloidal patchy polymers", **Phys. Rev. Lett.**, 110, 075501 (2013)
10. B. Capone, I. Coluzza, F. G. Lo Verso, C. N. Likos, R. Blaak, "Telechelic star polymers as self-assembling units from the molecular to the macroscopic scale", **Phys. Rev. Lett.**, 109, 238301 (2012)
11. D. Marzi, C. N. Likos, B. Capone, "Coarse graining of star polymer colloid nanocomposites", **J. Chem. Phys.**, 137, 014902 (2012)
12. B. Capone, I. Coluzza, J.-P. Hansen, "Competing micellar and cylindrical phases in semi-dilute diblock copolymer solution", **Soft Matter**, 6, 6075 (2010)
13. PhD Thesis "Coarse-graining polymer solutions in the semi-dilute regime" PhD awarded by the University of Cambridge, UK on the 27/11/2010

Date: May 2, 2018

Barbara Capone

## Lista Pubblicazioni

Letizia Chiodo

1. E. Baldini, A. Dominguez, L. Chiodo, E. Sheveleva, M. Yazdi-Rizi, C. Bernhard, A. Rubio, M. Chergui, "Anomalous Exciton Temperature Dependence in Rutile  $\text{TiO}_2$ ", *Phys. Rev. B* - RC (2017).
2. \*E. Baldini, L. Chiodo, A. Dominguez, M. Palummo, S. Moser, M. Yazdi-Rizi, G. Auböck, B. Mallett, H. Berger, A. Magrez, C. Bernhard, M. Grioni, A. Rubio, M. Chergui, "Strongly bound excitons in anatase  $\text{TiO}_2$  single crystals and nanoparticles", *Nat. Comm.*, 10.1038/ncomms14938 (2017) (autore principale parte computazionale).
3. \*Y. Zhihua, P. E. Trevisanutto, L. Chiodo, I. Santoso, A. R. Barman, T. C. Asmara, S. Dhar, A. Terentjevs, F. Della Sala, V. Olevano, T. Venkatesan, A. Rusydi, "Emerging giant resonant exciton induced by Ta substitution in anatase  $\text{TiO}_2$ : A tunable correlation effect", *Phys. Rev. B* 93, 205118 (2016) (co-primo autore).
4. \*L. Chiodo, T. E. Malliavin, L. Maragliano, G. Cottone, G. Ciccotti, "A structural model of the human  $\alpha 7$  nicotinic receptor in an open conformation", *Plos One* 10 (7), e0133011 (2015).
5. \*P. Gargiani, S. Lisi, M. G. Betti, A. Taleb, F. Bertran, P. Le Fevre, L. Chiodo, "Orbital dependent Rashba splitting and electron phonon coupling of 2D Bi phase floating on  $\text{Cu}(100)$  surface", *J. Chem. Phys.* 139, 184707 (2013).
6. M. Palummo, G. Giorgi, L. Chiodo, A. Rubio, and K. Yamashita "The Nature of Radiative Transitions in  $\text{TiO}_2$ -Based Nanosheets", *J. Phys. Chem. C* **116**, 18495- 18503 (2012).
7. G. Mallocci, L. Chiodo, A. Rubio, A. Mattoni, "Structural and Optoelectronic Properties of Unsaturated  $\text{ZnO}$  and  $\text{ZnS}$  Nanoclusters", *J. Phys. Chem. C*, **116**, 8741-8746 (2012).
8. \*L. Chiodo, L. A. Constantin, E. Fabiano, and F. Della Sala, "Nonuniform scaling applied to surface energies of transition metals", *Phys. Rev. Lett.* 108, 126402 (2012).
9. \*L. Chiodo, M. Salazar, A. H. Romero, S. Laricchia, F. Della Sala, and A. Rubio, "Structure, electronic and optical properties of  $\text{TiO}_2$  atomic clusters: an ab initio study", *J. Chem. Phys.* **135**, 244704 (2011) (doi: 10.1063/1.3668085).
10. G. Giorgi M. Palummo, L. Chiodo, and K. Yamashita, "Excitons at the (001) surface of anatase: Spatial behavior and optical signatures", *Phys. Rev. B* **84**, 073404 (2011) (BR).
11. \*L. Chiodo, J. M. García-Lastra, A. Iacomino, S. Ossicini, J. Zhao, H. Petek, A. Rubio, "Self-energy and excitonic effects in the electronic and optical properties of  $\text{TiO}_2$  crystalline phases", *Phys. Rev. B* 82, 045207 (2010).
12. L. Carbone, C. Nobile, M. De Giorgi, F. Della Sala, G. Morello, P.P. Pompa, M. Hytch, E. Snoeck, A. Fiore, I. R. Franchini, M. Nadasan, A. F. Silvestre, L. Chiodo, S. Kudera, R. Cingolani, R. Krahne and L. Manna, "Synthesis and Micrometer-Scale Assembly of Colloidal  $\text{CdSe/CdS}$  Nanorods Prepared by a Seeded Growth Approach", *Nano Lett.* 7, 2942 (2007).

Pubblicazioni in cui LC sia primo o co-primo autore, o autore principale della parte teorico-computazionale, e/o abbia supervisionato il lavoro computazionale e abbia scritto il lavoro, o sia il corresponding author, sono evidenziate con un asterisco\*

**Ph.D. Thesis title:** 'Ab initio study of electronic and optical properties of metallic surfaces with adsorbates'. Advisor: Prof. R. Del Sole.

Roue, 3-5-2018

Letizia Chiodo

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## Elenco delle pubblicazioni e della tesi di dottorato presentate

Tesi di dottorato:

1. Titolo della tesi (in lingua inglese): *Chiral phase transitions on quasi-1D frustrated spin systems*. Dottorato di Ricerca in Fisica, Università di Modena e Reggio Emilia, Modena, Relatori: Prof. Marco Affronte e Prof. Angelo Rettori – Certificazione Atto, data: 23/03/2004, n.registro: 200877059/D2, rilasciato da: Ufficio Post-Laurea - Esami di Stato Università di Modena e Reggio Emilia.

Pubblicazioni:

1. F. Cinti, A. Cappellaro, L. Salasnich, and T. Macrì;  
*Superfluid filaments of dipolar bosons in free space*;  
Physical Review Letters **119**, 215302 (2017)  
<https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.119.215302>
2. R. Diaz-Mendez, F. Mezzacapo, W. Lechner, F. Cinti, E. Babaev and G. Pupillo;  
*Glass Transitions in Monodisperse Cluster-Forming Ensembles: Vortex Matter in Type-1.5 Superconductors*;  
Phys. Rev. Lett. **118**, 067001 (2017)  
<https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.118.067001>
3. R. Diaz-Mendez, F. Mezzacapo, F. Cinti, W. Lechner, and G. Pupillo;  
*Monodisperse cluster crystals: Classical and quantum dynamics*;  
Physical Review E **92**, 052307 (2015)  
<http://journals.aps.org/pre/abstract/10.1103/PhysRevE.92.052307>
4. F. Cinti, M. Boninsegni, and T. Pohl;  
*Exchange-induced crystallization of soft core bosons*;  
New Journal of Physics **16**, 033038 (2014)  
<http://stacks.iop.org/1367-2630/16/033038>
5. F. Cinti, T. Macrì, W. Lechner, G. Pupillo, and T. Pohl;  
*Defect-induced supersolidity with soft-core Bosons*;  
Nat. Commun. **5**:3235 doi: 10.1038/ncomms4235 (2014)  
[http://www.nature.com/ncomms/2014/140204/ncomms4235/full/ncomms4235.html?WT.ec\\_id=NCOMMS-20140205](http://www.nature.com/ncomms/2014/140204/ncomms4235/full/ncomms4235.html?WT.ec_id=NCOMMS-20140205)
6. T. Macrì, F. Maucher, F. Cinti, and T. Pohl;  
*Elementary excitations of ultracold soft-core bosons across the superfluid-supersolid phase transition*;

- Physical Review A **87**, 061602(R) (2013)  
<http://journals.aps.org/prl/abstract/10.1103/PhysRevA.87.061602>
7. N. Henkel, F. Cinti, P. Jain, G. Pupillo, and T. Pohl;  
*Supersolid Vortex Crystals in Rydberg-dressed Bose-Einstein Condensates*;  
Physical Review Letters **108**, 265301 (2012)  
<https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.108.265301>
  8. P. Jain, F. Cinti, and M. Boninsegni;  
*Structure, Bose-Einstein condensation, and superfluidity of two-dimensional confined dipolar assemblies*;  
Physical Review B **84**, 014534 (2011)  
<https://journals.aps.org/prb/abstract/10.1103/PhysRevB.84.014534>
  9. F. Cinti, A. Rettori, and A. Cuccoli;  
*Vector chiral spin liquid phase in quasi-1d incommensurate helimagnets*;  
Physical Review B **83**, 174415 (2011)  
<https://journals.aps.org/prb/abstract/10.1103/PhysRevB.83.174415>
  10. F. Cinti, P. Jain, M. Boninsegni, A. Micheli, P. Zoller and G. Pupillo;  
*Supersolid droplet crystal in a dipole-blockaded gas*;  
Physical Review Letters **105**, 135301 (2010)  
<https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.105.135301>
  11. F. Cinti, A. Cuccoli, and A. Rettori,  
*Exotic Magnetic Structures in Ultrathin Helimagnetic Ho Films*;  
Physical Review B **78**, 020402(R) (2008)  
<https://journals.aps.org/prb/abstract/10.1103/PhysRevB.78.020402>
  12. F. Cinti, A. Rettori, M. G. Pini, M. Mariani, E. Micotti, A. Lascialfari, N. Papi-  
nutto, A. Amato, A. Caneschi, D. Gatteschi, and M. Affronte,  
*Two-step magnetic ordering in quasi-one-dimensional helimagnets: possible expe-  
rimental validation of Villain's conjecture about a chiral spin liquid phase*;  
Physical Review Letters **100**, 057203 (2008)  
<https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.100.057203>

Bologna, 27 aprile 2018



Fabio Cinti



## Elenco Pubblicazioni e Tesi di Dottorato

Laura Fanfarillo, Ph.D.

- [P1.] L. Fanfarillo, L. Benfatto, B. Valenzuela,  
*Orbital mismatch boosting nematic instability in iron-based superconductors*,  
Phys. Rev. B **97**, 121109(R) (2018).
- [P2.] L. Fanfarillo, G. Giovannetti, M. Capone and E. Bascones,  
*Nematicity at the Hund's metal crossover in iron superconductors*,  
Phys. Rev. B **95**, 144511 (2017).
- [P3.] L. Fanfarillo, J. Mansart, P. Toulemonde, H. Cercellier, P. Le Fevre, F. Bertran, B. Valenzuela, L. Benfatto, and V. Brouet,  
*Orbital-dependent Fermi Surface shrinking as a fingerprint of nematicity in FeSe*,  
Phys. Rev. B **94**, 155138 (2016).
- [P4.] L. Fanfarillo and E. Bascones,  
*Electronic correlations in Hund metals*,  
Phys. Rev. B **92**, 075136 (2015).
- [P5.] L. Fanfarillo, A. Cortijo, B. Valenzuela,  
*Spin-orbital interplay and topology in the nematic phase of iron pnictides*,  
Phys. Rev. B **91**, 214515 (2015).
- [P6.] L. Fanfarillo, E. Cappelluti, C. Castellani, L. Benfatto,  
*Unconventional Hall Effect in Pnictides from Interband Interactions*,  
Phys. Rev. Lett. **109**, 096402 (2012).
- [P7.] L. Fanfarillo, L. Benfatto, C. Castellani,  
*Current-current Fermi-liquid corrections to the superconducting fluctuations on conductivity and diamagnetism*,  
Phys. Rev. B **85**, 024507 (2012).
- [P8.] L. Fanfarillo, L. Benfatto,  
*Anisotropy of the superconducting fluctuations in multiband superconductors: the case of LiFeAs*,  
Supercond. Sci. Technol. **27**, 124009 (2014), invited paper for a focus issue on Multicomponent Superconductivity
- [P9.] M. Marciani, L. Fanfarillo, C. Castellani, L. Benfatto,  
*Legget modes in Fe-based superconductors as a probe of Time Reversal Symmetry Breaking*,  
Phys. Rev. B **88**, 214508 (2013).
- [P10.] L. Fanfarillo, L. Benfatto, S. Caprara, C. Castellani, M. Grilli,  
*Theory of fluctuation conductivity from interband pairing in pnictide superconductors*,  
Phys. Rev. B **79**, 172508 (2009).



- [P11.] A. Ronchi, P. Franceschini, L. Fanfarillo, P. Homin, M. Menghini, S. Peli, G. Ferrini, F. Banfi, F. Cilento, A. Damascelli, F. Parmigiani, J-P Locquet, M. Fabrizio, M. Capone and C. Giannetti, *Ultrafast orbital manipulation and Mott physics in multi-band correlated materials*, Proc. SPIE 10530, 105300V (2018)
- [P12.] L. Fanfarillo, M. Mori, M. Campetella, M. Grilli, S. Caprara, *Glue function of optimally and overdoped cuprates from inversion of the Raman spectra*, Journal of Physics: Condensed Matter **28**, 065701 (2016).
- [PhDThesis.] Ph.D. thesis. Sapienza - University of Rome  
L. Fanfarillo, *Transport properties in multichannel systems*,

Trieste, 2 Maggio 2018

Laura Fanfarillo



**ALLEGATO B**

**DICHIARAZIONI SOSTITUTIVE DI CERTIFICAZIONI**  
(Art. 46 D.P.R. n.445/2000)

**DICHIARAZIONI SOSTITUTIVE DELL'ATTO DI NOTORIETA'**  
(Art. 19 e 47 D.P.R. n.445/2000)

Il sottoscritto Cosimo Gorini, nato a [redacted] il [redacted]

[redacted] consapevole che le dichiarazioni mendaci sono punite ai sensi del codice penale e delle leggi speciali in materia

**DICHIARA:**

di essere autore o coautore di ogni e ciascuna pubblicazione di cui alla lista seguente contenente l'elenco delle pubblicazioni e della tesi di dottorato presentate ai fini della valutazione.

Monaco di Baviera, 2 Maggio 2018



**Elenco delle pubblicazioni e della tesi di dottorato presentate ai fini della  
valutazione**

1. J. Ziegler, R. Kozlovsky, C. Gorini, M.-H. Liu, S. Weishäupl, H. Maier, R. Fischer, D. A. Kozlov, Z. D. Kvon, N. Mikhailov, S. A. Dvoretzky, K. Richter, and D. Weiss, "*Probing spin helical surface states in topological HgTe nanowires*", Physical Review B **97**, 0335157 (2018).
2. G. V. Karnad, C. Gorini, K. Lee, T. Schulz, R. Lo Conte, A. W. J. Wells, D.-S. Han, K. Shahbazi, J.-S. Kim, T. A. Moore, H. J. M. Swagten, U. Eckern, R. Raimondi, and M. Kläui, "*Evidence for phonon skew scattering in the spin Hall effect of platinum*", Physical Review B (Rapid) **97**, 100405(R) (2018).
3. C. Gorini, A. Maleki Sheikhabadi, K. Shen, I. Tokatly, G. Vignale and R. Raimondi, "*Theory of current-induced spin polarization in an electron gas*", Physical Review B **95**, 205424 (2017).

4. P. Reck, C. Gorini, A. Goussev, V. Krueckl, M. Fink and K. Richter, "*Dirac quantum time mirror*", Physical Review B **95**, 165421 (2017).
5. M. Liu, C. Gorini and K. Richter, "*Creating and Steering Highly Directional Electron Beams in Graphene*", Physical Review Letters **118**, 066801 (2017).
6. C. Gorini, U. Eckern and R. Raimondi, "*Spin Hall Effects Due to Phonon Skew Scattering*", Physical Review Letters **115**, 076602 (2015).
7. R. Bosisio, C. Gorini, G. Fleury and J. Pichard, "*Gate-modulated thermopower of disordered nanowires: II. Variable-Range Hopping Regime*", New Journal of Physics **16**, 095005 (2014).
8. C. Gorini, R. Jalabert, W. Szewc, S. Tomsovic and D. Weinmann, "*Theory of scanning gate microscopy*", Physical Review B **88**, 035406 (2013).
9. C. Gorini, R. Raimondi and P. Schwab, "*Onsager Relations in a Two-Dimensional Electron Gas with Spin-Orbit Coupling*", Physical Review Letters **109**, 246604 (2012).
10. C. Gorini, P. Schwab, R. Raimondi and A. Shelankov, "*Non-Abelian gauge fields in the gradient expansion: Generalized Boltzmann and Eilenberger equations*", Physical Review B **82**, 195316 (2010).
11. C. Gorini, P. Schwab, M. Dzierzawa and R. Raimondi, "*Spin polarizations and spin Hall currents in a two-dimensional electron gas with magnetic impurities*", Physical Review B **78**, 125327 (2008).
12. R. Raimondi, C. Gorini, P. Schwab and M. Dzierzawa, "*Quasiclassical approach to the spin Hall effect in the two-dimensional electron gas*", Physical Review B **74**, 035340 (2006).
13. C. Gorini, "*Quasiclassical methods for spin-charge coupled dynamics in low-dimensional systems*", Tesi di dottorato, Universität Regensburg (DE), cotutela con Università Roma Tre (2009).

*Handwritten signatures and marks:*  
 

**LISTA DELLE PUBBLICAZIONI SCIENTIFICHE SELEZIONATE AI FINI DELLA  
VALUTAZIONE E DELLA TESI DI DOTTORATO**

Le pubblicazioni e la tesi di dottorato sono riportate in formato PDF nella cartella PUBBLICAZIONI/

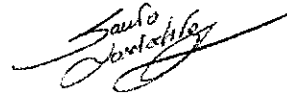
- 1) **S. Laricchia**, E. Fabiano, F. Della Sala, Frozen density embedding with hybrid functionals, *J. Chem. Phys.* **133**, 164111 (2010);  
[nome file: ARTICOLO\_1/JCP\_133\_164111\_2010.pdf  
supplementary materials: ARTICOLO\_1/suppl\_mat\_JCP\_133\_164111\_2010.pdf]
- 2) Lucian A. Constantin, E. Fabiano, **S. Laricchia**, and F. Della Sala, Semiclassical Neutral Atom as a Reference System in Density Functional Theory, *Phys. Rev. Lett.* **106**, 186406 (2011);  
[nome file: ARTICOLO\_2/PRL\_106\_186406\_2011.pdf  
supplementary materials: ARTICOLO\_2/suppl\_mat\_PRL\_106\_186406\_2011.pdf]
- 3) **S. Laricchia**, E. Fabiano, Lucian A. Constantin, and F. Della Sala, Generalized Gradient Approximations of the Noninteracting Kinetic Energy from the Semiclassical Atom Theory: Rationalization of the Accuracy of the Frozen Density Embedding Theory for Nonbonded Interactions, *J. Chem. Theory Comput.* **7** (8), 2439 (2011);  
[nome file: ARTICOLO\_3/JCTC\_7\_2439\_2011.pdf  
supplementary materials: ARTICOLO\_3/suppl\_mat\_JCTC\_7\_2439\_2011.pdf]
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Luogo e data:  
Londra, 03/05/2018

Dichiarante:



*Lepori*

21/04/2018

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## TESI DOTTORATO

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"Water at the interface with molecules of biological interest: from sugars to proteins."

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Salt Lake City, 23/04/2018

Firma

*Laura Lupi*

*MR*

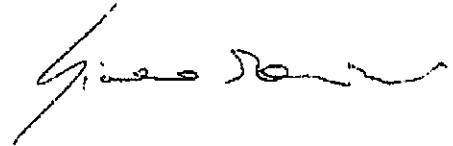
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April 26, 2018



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Candidata: Margherita Marsili

Bando: RTD B 02/B2, S.S.D. FIS/03 (Gazzetta Ufficiale n. 27 (anno 159) 3 aprile 2018)

1. M. Marsili, E. Mosconi, F. De Angelis, P. Umari "Large scale GW-BSE calculations with N3 scaling: excitonic effects in dye sensitised solar cells", Phys. Rev. B 95, 075415 (2017)
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Palaiseau 02/05/2018

*Margherita Marsili*

*MR F*

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Data: 21/04/2-18



## Lista delle 12 pubblicazioni e della Tesi di Dottorato

Matteo Paoluzzi\*

Department of Physics and Syracuse Soft & Living Matter Program, Syracuse University, Syracuse NY 13244, USA

### Scientific publications in refereed journals or refereed proceedings

1. M. Paoluzzi, L. Leuzzi, and A. Crisanti, Phys. Rev. Lett. 104, 120602 (2010).  
*Thermodynamic first order transition and inverse freezing in a 3D spin-glass.*
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3. M. Paoluzzi, R. Di Leonardo, and L. Angelani, Journal of Physics: Condensed Matter 45 (41), 415102 (2013).  
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\* equal contribution
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\* equal contribution

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Ph.D. Thesis

1. M. Paoluzzi, Università degli Studi "Roma Tre" (2012)  
*Multiscale models in Condensed Matter.*

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SYRACUSE, NY, USA

30/04/2018

Matteo Paoluzzi

MP



DICHIARAZIONI SOSTITUTIVE DI CERTIFICAZIONI  
(art. 46 D.P.R. n.445/2000)

DICHIARAZIONI SOSTITUTIVE DELL'ATTO DI NOTORIETA'  
(art. 19 e 47 D.P.R. n.445/2000)

Il sottoscritto

COGNOME PASTORE  
(per le donne indicare il cognome da nubile)  
NOME RAFFAEL

consapevole che le dichiarazioni mendaci sono punite ai sensi del Codice penale e delle leggi speciali in materia

DICHIARA:

che le sottoelencate pubblicazioni e la tesi di dottorato, allegate in formato digitale alla presente domanda e di seguito elencate (punto I), sono conformi agli originali.

DICHIARA inoltre:

di essere in possesso dei titoli di seguito elencati (punto II).

I) ELENCO DELLE PUBBLICAZIONI E DELLA TESI DI DOTTORATO PRESENTATE

\*=corresponding author

- 1) Z. Zheng, F. Li, Jun Liu, R. Pastore, G. Raos, Y. Wu and L. Zhang, "Effects of Chemically Heterogeneous Nanoparticles on Polymer Dynamics: Insights from Molecular Dynamics Simulations", *Soft Matter* 14 (2018), pp.1219-1226. DOI: 10.1039/c7sm02414b
- 2) R. Pastore\*, G. Pesce, A. Sasso and M. Pica Ciamarra, "Cage Size and Jump Precursors in Glass-Forming Liquids: Experiment and Simulations", *The Journal of Physical Chemistry Letters* 8 (2017), pp. 1562-1568. DOI: 10.1021/acs.jpclett.7b00187
- 3) R. Pastore\*, G. Pesce and M. Caggioni, "Differential Variance Analysis: a direct method to quantify and visualize dynamic heterogeneities", *Scientific Reports* 7, 43496 (2017), pp.1-9. DOI: 10.1038/srep43496
- 4) M. Casalegno, R. Pastore, J. Idé, R. Po and G. Raos\*, "Origin of Charge Separation at Organic Photovoltaic Heterojunctions: A Mesoscale Quantum Mechanical View", *The Journal of Physical Chemistry C* 121 (2017), pp.16693-16701. DOI: 10.1021/acs.jpcc.7b03640
- 5) M. Pica Ciamarra, R. Pastore\* and A. Coniglio\*, "Particle jumps in structural glasses", *Soft Matter* 12 (2016), pp.358-366. Review article. DOI: 10.1039/C5SM01568E
- 6) R. Pastore\* and G. Raos\*, "Glassy dynamics of a polymer monolayer on a heterogeneous disordered substrate", *Soft Matter* 11 (2015), pp.8083-8091. DOI: 10.1039/C5SM01440A
- 7) R. Pastore\*, A. Coniglio and M. Pica Ciamarra, "Spatial correlations of elementary relaxation events in glass-forming liquids", *Soft Matter* 11 (2015), pp.7214-7218. DOI: 10.1039/C5SM01510C

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- 8) R. Pastore\*, A. Coniglio and M. Pica Ciamarra, "Dynamic phase coexistence in glass-forming liquids", Scientific Reports 5, 11770 (2015), pp.1-10. DOI: 10.1038/srep11770
  - 9) R. Pastore\*, G. Pesce, M. Pica Ciamarra and A. Sasso, "Connecting short and long time dynamics in hard-sphere-like colloidal glasses", Soft Matter, 11 (2015), pp.622-626. DOI: 10.1039/C4SM02147A
  - 10) R. Pastore\*, A. Coniglio and M. Pica Ciamarra, "From cage-jump motion to macroscopic diffusion in supercooled liquids", Soft Matter 10 (2014), pp.5724-5728. DOI: 10.1039/C4SM00739E
  - 11) R. Pastore\*, M. Pica Ciamarra, A. de Candia and A. Coniglio, "Dynamical Correlation Length and Relaxation Processes in a Glass Former", Physical Review Letters 107, 065703 (2011), pp.1-4. DOI: 10.1103/PhysRevLett.107.065703
  - 12) M. Pica Ciamarra\*, R. Pastore, M. Nicodemi and A. Coniglio, "Jamming phase diagram for frictional particles", Physical Review E 84, 041308 (2011), pp.1-10. DOI: 10.1103/PhysRevE.84.041308
- **TESI DI DOTTORATO:** R. Pastore, "Jamming transition in thermal and non-thermal systems", <http://www.fedoa.unina.it/8617/> (2011), Tutor: Prof. A. Coniglio.

## II) ELENCO DEI TITOLI

a) dottorato di ricerca o equipollente conseguito in Italia o all'estero (per i settori interessati il diploma di specializzazione medica o equivalente)

Dicembre 2008 - 21/12/2011: **Dottorato (Ph.D.)** in "Fisica Fondamentale ed Applicata" (XXIV Ciclo) presso l'Università degli Studi di Napoli Federico II, con giudizio: Ottimo. Tesi di Dottorato: "*Jamming transition in thermal and non-thermal systems*", Tutor: Prof. A. Coniglio.

b) attività didattica a livello universitario in Italia o all'estero:

- Ottobre - Dicembre 2018: **Corso di Esercitazioni di Fisica** per gli studenti del corso di Laurea in Farmacia, Università di Napoli Federico II.
- Marzo - Agosto 2016: **Supervisione** di uno studente "graduate", S. Shahsavari (MIT, Boston, USA) e "undergraduate", E. Bruckner (Case Western Reserve University, Cleveland, USA) durante la loro "internship" presso i laboratori Procter&Gamble di Cincinnati (Ohio, USA).
- 11/6/2012: **Seminario**, "Fractal suggestions for designers" per gli studenti della Laurea Magistrale in Architettura e Design di Napoli presso la Seconda Università di Napoli "SUN".
- 17/5/2011: **Seminario**, "The Jamming transition for granular materials", presso il Dipartimento di Ingegneria Chimica, Università di Napoli "Federico II" e per gli studenti del corso di "Ingegneria dei Sistemi Colloidali".
- Gennaio - Dicembre 2010: In qualità di titolare di una borsa annuale per l'insegnamento, "Assegni per l'incentivazione delle attività di tutorato a.a. 2010/2011", presso l'Università di Napoli Federico II ho tenuto i seguenti corsi e attività:
- Marzo - Giugno 2010: **Corso di Tutorato in Fisica 1** per gli studenti delle lauree triennali in Chimica e Informatica, Università di Napoli "Federico II".
- Gennaio - Febbraio 2010: **Corso di Tutorato Istituzioni di Analisi Matematica** per gli studenti della Laurea triennale in Ottica e Optometria dell'Università di Napoli Federico II.
- Gennaio - Dicembre 2010: **Tutorato individuale** di studenti dell'Università di Napoli Federico II.

c) attività di formazione o di ricerca presso qualificati istituti italiani o stranieri:

- 18/12/2017 - Oggi: **Ricercatore Universitario RTD-A** presso Dipartimento di Ingegneria Chimica, dei Materiali e della Produzione Industriale (DICMAPI), Università degli Studi di Napoli Federico II. Settore concorsuale: 09/D2. Settore scientifico disciplinare: ING-IND/23.
- 01/02/2015 - 16/12/2015: **Assegnista di Ricerca Postdoc** presso CNR-SPIN, U.O.S. Napoli (Laboratorio Congiunto: "CNR- NTU Singapore"). Responsabile: Dr. A. Fierro. Tematiche: Simulazioni di Dinamica

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- 01/02/2015 – 16/12/2015: **Assegnista di Ricerca Postdoc** presso **CNR-SPIN, U.O.S. Napoli** (Laboratorio Congiunto: "CNR- NTU Singapore"). Responsabile: Dr. A. Fierro. Tematiche: Simulazioni di Dinamica Molecolare e Browniana di liquidi molecolari sottoraffreddati, sospensioni colloidali dense e polimeri nano compositi. Simulazioni Monte Carlo e calcoli quanto-meccanici per la generazione e il trasporto di corrente in 'organic photovoltaic heterojunction'. Analisi e modellazione dei dati derivanti dalle simulazioni e da esperimenti di video-microscopia ottica su sospensioni colloidali. Tali analisi sono state realizzate per mezzo di programmi in C++ e Python sviluppati da me medesimo.
- Novembre 2017-Febbraio 2018: **Visiting Scientist** presso il Dipartimento di Biotecnologie Mediche e Medicina Traslazionale dell'Università degli Studi di Milano. Provvedimento approvato dal Consiglio di Dipartimento, con verbale del 29/9/2017, nell'ambito di una collaborazione con il Prof. R. Cerbino. Tematiche: Analisi e modellazione dei dati derivanti da esperimenti su sospensioni colloidali e schiume, acquisiti grazie a video-microscopia digitale.
- Novembre 2017-Gennaio 2018: **Visiting Scientist** presso il Dipartimento di Chimica, Materiali e Ingegneria Chimica "G. Natta" del Politecnico di Milano. Lettera di invito ricevuta dal Direttore di Dipartimento, Prof. M. Masi, in data 18/9/2017, nell'ambito di una collaborazione con il Prof. G. Raos. Tematiche: Simulazioni di Dinamica Molecolare e Browniana di polimeri nano compositi e sospensioni colloidali. Analisi statistica e modellazione dei dati.
- 1/3/2016 - 31/8/2016: **Visiting Scholar** invitato presso **University of Cincinnati (UC)** e **Laboratori Procter&Gamble (P&G)** di Cincinnati (Ohio, USA) nell'ambito di una collaborazione con il Dr. M. Caggioni (Senior Engineer presso P&G). Posizione finanziata da UC e P&G.
- 12-28 Ottobre 2015: **Ospite scientifico a Singapore**, presso **Nanyang Technological University (NTU)**, nell'ambito del Laboratorio Congiunto: "CNR- NTU Singapore".
- 1/1/2012 - 31/12/2014: **Assegnista di Ricerca Postdoc** presso **CNR-SPIN, U.O.S. Napoli**. Responsabile: Dr. M. Pica Ciamarra (attualmente Associate Professor presso NTU Singapore).
- 29 Giugno - 9 Luglio 2010: **International Summer School Complex materials in physics and biology**, Società Italiana di Fisica, Varenna.
- 31 Agosto - 11 Settembre 2009: **International Summer School Fundamental problems in Statistical Physics XII**, Leuven (Belgio).
- Gennaio 2006 - 28/3/2008: **Laurea Specialistica in Fisica** presso l'Università degli Studi di Napoli Federico II, con voto 110/110 E LODE. Tesi di Laurea: "*Reologia e Jamming nella materia granulare*", Relatore Prof. A. Coniglio. Tematiche: Simulazioni di dinamica molecolare e analisi di sistemi granulari.
- Ottobre 2001 - 14/12/2005: **Laurea Triennale in Fisica** conseguita presso l'Università degli Studi di Napoli Federico II, con voto 110/110. Tesi di Laurea: "*Violazione della simmetria CP nel sistema dei K neutri e misura di  $Re(\epsilon'/\epsilon)$  presso una 'fabbrica di  $\Phi'$* ", Relatore Prof. M. Napolitano.
- Febbraio - Agosto 2004: **Progetto Erasmus** presso Istituto de Astrofisica de Canarias, Universidad de La Laguna, Tenerife (Spagna).
- 1996 - 2001: **Diploma di Maturità Classica** conseguito presso il Liceo-Ginnasio Jacopo Sannazzaro con voto 100/100.

f) organizzazione, direzione e coordinamento di gruppi di ricerca nazionali e internazionali, o partecipazione agli stessi:

- Maggio 2017 - Oggi: **Principal Investigator** del progetto "Characterizing liquid fabric enhancers through dynamic heterogeneities: simulations and experiment". Fase iniziale del progetto supportata da Procter&Gamble con un Grant di € 9000. Istituzioni coinvolte nella collaborazione: Università di Napoli Federico II, P&G Brussels, P&G Cincinnati, Politecnico di Milano.
- Marzo - Agosto 2016: **Grant** di \$16000 da University of Cincinnati e Procter&Gamble a supporto della mia posizione di Visiting Scholar a Cincinnati (Ohio, USA). In questa posizione, ho svolto come **Principal Investigator** un progetto dedicato alla caratterizzazione di sospensioni colloidali dense basata sull'analisi di video-microscopia digitale. Istituzioni coinvolte nella collaborazione: CNR-SPIN, P&G Cincinnati, University of Cincinnati, Università di Napoli Federico II.
- 2015 - Oggi: **Principal Investigator** del progetto "Charge separation and charge transport in hybrid solar cells", risultato vincitore della call CNR-SPIN SEED 2014 e finanziato con un Grant di €12000. Istituzioni coinvolte

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- 2018 (attualmente in revisione): **Partecipazione** al progetto PRIN 2018 – Linea Giovani, con Dr. R. Pasquino (coordinatore nazionale, Università di Napoli Federico II), Dr. F. Romano (coordinatore locale, Università di Venezia), Dr. N. Gnan (coordinatore locale, CNR-ISC Roma), Dr. G. Zanchetta (coordinatore locale, Università di Milano).
- 2015 - Oggi: **Partecipazione** al Laboratorio Congiunto CNR–NTU Singapore, per il progetto "Amorphous materials for energy harvesting applications". Finanziato dal CNR con un Grant di k€ 150. PIs: Dr. A. Fierro (CNR-SPIN), Prof. M. Pica Ciamarra (NTU Singapore).
- 2011 - 2015: **Partecipazione** al progetto MIUR-FIRB RBFR081IUK "Unjamming transition in granular systems and earthquake precursors: theory, experiments and simulations". PI: Dr. M. Pica Ciamarra (CNR-SPIN).
- 2009 - 2012: **Partecipazione** al progetto PRIN 2009 "Microscopic origin of the stick-slip instability in granular systems: theory, simulations and experiments". PI: Prof. A. Coniglio (Università di Napoli Federico II).
- 2017 - Oggi: **Collaborazione** con il Prof. R. Cerbino (Università di Milano): Studio del rilassamento "stretched and compressed exponential" in schiume e vetri colloidali, e, studio di eterogeneità dinamiche e loro dipendenza dalla lunghezza d'onda in vetri colloidali, basati su video-microscopia digitale.
- 2017 - Oggi: **Collaborazione** con il gruppo del Prof. J. Liu (Beijing University of Chemical Technology) e con il Prof. G. Raos (Politecnico di Milano): Studio numerico di polimeri nano-compositi.
- 2014 - Oggi: **Collaborazione** con il gruppo del Prof. G. Raos (Politecnico di Milano): Studio numerico di polimeri adsorbiti su/confinati tra superfici nanostrutturate.
- 2016 - oggi: **Collaborazione** con il gruppo del Dr. M. Ribera D'Alcalá (Stazione Zoologica Dhorn, Napoli): Studio della dinamica di una specie di plankton attraverso analisi di traiettorie 3d ottenute grazie a lenti telecentriche.
- 2013 - 2017: **Collaborazione** con il gruppo del Prof. A. Sasso (Università di Napoli Federico II) e con il Prof. M. Pica Ciamarra (NTU Singapore): Studio della dinamica di vetri colloidali attraverso analisi di traiettorie ottenute da video-microscopia digitale e confronto con simulazioni numeriche.

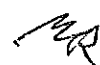
h) relatore a congressi e convegni nazionali e internazionali:

- 17-20 Aprile 2018: Annual European Rheology Conference, AERC 2018, Sorrento (Italia). **Talk:** "Dense vesicle suspensions: relaxation processes and dynamic heterogeneities".
- 5-9 Febbraio 2018: Flowing Matter 2018 (organized by Cost Action MP1305 Flowing Matter), Lisbona (Portogallo). **Talk:** "Cage Size and Jump Precursors in Glass-Forming Liquids: Experiment and Simulations".
- 21 - 23 Giugno 2017: Rheology of gel networks: combining experimental computational and theoretical insights (CECAM Workshop), Lione (Francia), **Poster:** "Differential Variance Analysis of soft glassy materials: a direct method to quantify and visualize structural relaxation and dynamic heterogeneities".
- 22 - 26 Maggio 2017: Fluids and Structures: Interaction and Modeling (organized by Cost Action MP1305 Flowing Matter), Napoli, **Talk:** "Structural relaxation and dynamic heterogeneities in soft materials: a simple experimental approach".
- 24/11/2016: III Workshop Ph.D. Complex Fluids School (organized by Procter&Gamble e Università di Napoli Federico II), Napoli, **Talk:** "Dynamic heterogeneities in complex fluids: a simple experimental approach".
- 4 - 9 Settembre 2016: 30th Conference of the European Colloid and Interface Society, Roma, **Talk:** "Many facets of intermittent dynamics in colloidal and molecular glasses".
- 5 - 8 Giugno 2016: 90th ACS Colloid & Surface Science Symposium, Harvard University, Boston (USA), **Talk:** "Many facets of intermittent dynamics in colloidal and molecular glasses".

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- 21 - 23 Luglio 2015: The role of local structure in dynamical arrest (CECAM Workshop), Mainz (Germania), **Talk:** "Cage-jump motion reveals universal dynamics and non-universal structural features in glass forming liquid".
- 4 - 7 Maggio 2015: International Workshop on Dynamics in Viscous Liquids, Montpellier (Francia), **Poster:** "Hopping and dynamical phase coexistence in supercooled liquids".
- 22 - 25 Marzo 2015: XIV International Workshop on Complex Systems, Fai della Paganella (Trento), **Talk:** "Hopping and dynamic phase coexistence in glass formers".
- 17 - 18 Settembre 2014: Italian Soft days 2014, Roma: **Talk:** "From cage-jump motion to macroscopic dynamics in glass formers".
- 8 - 13 Settembre 2014: Critical Phenomena in Random and Complex Systems, Capri (Italy), **Poster:** "From cage-jump motion to macroscopic dynamics in glass formers".
- 21 - 26 Luglio 2013: 7th International Meeting on Relaxations in Complex Systems, Barcellona (Spagna), **Due Poster:** i) "Cages and Jumps in supercooled liquids"; ii) "Dynamical Correlation Length and Relaxation Processes in a Glass Former".
- 2 - 5 Giugno 2012: Frontiers in Statistical Physics and Complex Systems, Catania: **Poster:** "Dynamical Correlation Length and Relaxation Processes in a Glass Former".
- 18 - 22 Marzo 2012: XIII Andalo workshop on complex systems, Andalo (Trento), **Talk:** "Dynamical Correlation Length and Relaxation Processes in a Glass Former".
- 15 - 18 Marzo 2010: XII Andalo workshop on complex systems, Andalo (Trento): **Talk:** "The role of friction in the Jamming transition".
- Gennaio 2010: Journées de Physique Statistique 2010, ESPCI, Parigi (Francia), **Talk:** "Jamming phase diagram for frictional particles".

i) premi e riconoscimenti nazionali e internazionali per attività di ricerca:

- Settembre 2017: L'articolo, *M. Casalegno, R. Pastore et al., J. Phys. Chem. C 121, 16693 (2017)* è incluso nella lista dei "most read articles" di the Journal of Physical Chemistry C durante i trenta giorni precedenti.
- Aprile 2017: **Comunicato stampa** del CNR relativo all'articolo, *R. Pastore et al., Sci. Rep. 7, 43496 (2017)*: <https://www.cnr.it/it/comunicato-stampa/7427/that-s-the-way-soft-matter-relaxes>
- Maggio 2017: **News** sul sito ufficiale della University of Cincinnati relativo all'articolo, *R. Pastore et al., Sci. Rep. 7, 43496 (2017)*: <http://www.uc.edu/news/NR.aspx?id=25052>
- Marzo 2017: **News** sul sito ufficiale della Università di Napoli Federico II relativo all'articolo, *R. Pastore et al., Sci. Rep. 7, 43496 (2017)*: <http://bit.ly/2nLm8SQ>
- Marzo 2017: **News** sul sito ufficiale dell'Istituto CNR-SPIN relativo all'articolo, *R. Pastore et al., Sci. Rep. 7, 43496 (2017)*: <http://www.spin.cnr.it/index.php/component/content/article/34-banner-news/208-dva>
- 2016: L'articolo, *R. Pastore et al., Sci. Rep. 5, 11770 (2015)*, è selezionato per gli **Highlights 2015** dell'Istituto CNR-SPIN: <http://www.spin.cnr.it/images/documents/spin-scirep-2014-2015.pdf>
- Ottobre 2014: **Vincitore** del concorso CNR-SPIN SEED 2014 con il progetto "Charge separation and charge transport in hybrid solar cells": <http://www.spin.cnr.it/index.php/seedprojects>
- 2012: L'articolo, *R. Pastore et al., Phys. Rev. Lett. 107, 065703 (2011)*, è selezionato per gli **Highlights 2011** dell'Istituto CNR-SPIN: <http://www.spin.cnr.it/index.php/highlights-2011>
- Novembre 2009: **Vincitore** di una borsa annuale per l'insegnamento "Assegni per l'incentivazione delle attività di tutorato a.a. 2010/2011", presso l'Università di Napoli Federico II.
- Dicembre 2008: **Vincitore** di una borsa di Dottorato in Fisica presso Università di Napoli Federico II.
- Ottobre 2008: **Vincitore** di una borsa di Dottorato in Scienze Fisiche delle Materia presso Università di Roma Tre-CNISM (non accettata).

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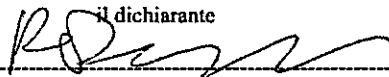
*R. Pastore*

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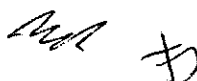
- Settembre 2008: **Vincitore** di una borsa di Dottorato in Fisica (Beca Apif) presso Universitat de Barcelona (Spagna) (non accettata).
- 2003: **Vincitore** di una borsa di studio Erasmus.
- 2006: **Vincitore** di un premio nel concorso "Diffusione cultura scientifica" dell'Università di Napoli Federico II.

Luogo e data NAPOLI, 02/05/2018

il dichiarante  


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## Elenco delle pubblicazioni presentate

- 1) *Charge migration in XUV photoexcited phenylalanine: a first-principles real-time Green's function study*,  
E. Perfetto, D. Sangalli, A. Marini and G. Stefanucci,  
J. Chem. Phys. Lett. **9**, 1353 (2018).
- 2) *Charge separation in donor-C60 complexes with real-time Green's functions: The importance of nonlocal correlations*,  
E. V. Bostrom, A. Mikkelsen, C. Verdozzi, E. Perfetto, and G. Stefanucci,  
Nano Letters **18**, 785 (2018).
- 3) *First-principles approach to excitons in time-resolved and angle-resolved photoemission spectra*  
E. Perfetto, D. Sangalli, A. Marini and G. Stefanucci,  
Phys. Rev. B **94**, 245303 (2016)
- 4) *Nonequilibrium Bethe-Salpeter equation for transient photoabsorption spectroscopy*  
E. Perfetto, D. Sangalli, A. Marini and G. Stefanucci,  
Phys. Rev. B **92**, 205304 (2015).
- 5) *First-principles nonequilibrium Green's-function approach to transient photoabsorption: Application to atoms*  
E. Perfetto, A. -M. Uimonen, R. van Leeuwen and G. Stefanucci,  
Phys. Rev. A **92**, 033419 (2015).
- 6) *Time-dependent Landauer-Büttiker formula: Application to transient dynamics in graphene nanoribbons*  
R. Tuovinen, E. Perfetto, G. Stefanucci, R. van Leeuwen.  
Phys. Rev. B **89**, 085131 (2014).
- 7) *Charge dynamics in molecular junctions: Nonequilibrium Green's function approach made fast*  
S. Latini, E. Perfetto, A.-M. Uimonen, R. van Leeuwen, and G. Stefanucci.  
Phys. Rev. B **89**, 075306 (2014).
- 8) *Dynamical Formation and Manipulation of Majorana Fermions in Driven Quantum Wires in Contact with a Superconductor*  
E. Perfetto,  
Phys. Rev. Lett. **110**, 087001 (2013).

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9) *Correlation induced memory effects in the transport properties of low dimensional systems,*

E. Perfetto , G. Stefanucci and M. Cini,  
Phys. Rev. Lett. **105**, 156802 (2010).

10) *Time-dependent quantum transport with superconducting leads: Kohn-Sham formulation and propagation scheme ,*

G. Stefanucci, E. Perfetto and M. Cini,  
Phys. Rev. B **81**, 115446 (2010).

11) *Quantum Hall Effect in Carbon Nanotubes and Curved Graphene Stripes,*

E. Perfetto, J. Gonzalez, F. Guinea, S. Bellucci and P. Onorato,  
Phys. Rev. B **76**, 125430 (2007).

12) *Time-Dependent Evolution of Two Coupled Luttinger Liquids,*

E. Perfetto,  
Phys. Rev. B **74**, 205123 (2006).

Roma, 26/04/2018

Dr Enrico Perfetto



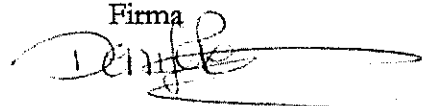


## Elenco pubblicazioni e tesi di dottorato presentate

- **D. Perrone**, O. Alexandrova, O. W. Roberts, S. Lion, C. Lacombe, A. Walsh, M. Maksimovic, I. Zouganelis, *Coherent structures at ion scales in fast solar wind: Cluster observations*, **The Astrophysical Journal** 849, 49 (2017);
- S. Servidio, A. Chasapis, W. H. Matthaeus, **D. Perrone**, F. Valentini, T. N. Parashar, P. Veltri, *Magnetospheric multiscale observation of plasma velocity-space cascade: Hermite representation and theory*, **Physical Review Letters** 119, 205101 (2017);
- **D. Perrone**, O. Alexandrova, A. Mangeney, M. Maksimovic, C. Lacombe, V. Rakoto, J. C. Kasper, D. Jovanovic, *Compressive coherent structures at ion scales in the slow solar wind*, **The Astrophysical Journal** 826, 196 (2016);
- S. Servidio, F. Valentini, **D. Perrone**, A. Greco, F. Califano, W.H. Matthaeus, P. Veltri, *A kinetic model of plasma turbulence*, **Journal of Plasma Physics** 81, 325810107 (2015);
- F. Valentini, S. Servidio, **D. Perrone**, F. Califano, W.H. Matthaeus, P. Veltri, *Hybrid Vlasov-Maxwell simulations of two-dimensional turbulence in plasmas*, **Physics of Plasmas**, 21, 082307 (2014);
- **D. Perrone**, F. Valentini, S. Servidio, S. Dalena, P. Veltri, *Analysis of intermittent heating in a multi-component turbulent plasma*, **European Physical Journal D** 68, 209 (2014);
- **D. Perrone**, S. Bourouaine, F. Valentini, E. Marsch, P. Veltri, *Generation of temperature anisotropy for alpha particle velocity distributions in the solar wind at 0.3 AU: Vlasov simulations and Helios observations*, **Journal of Geophysical Research** 119, 2400 (2014);
- **D. Perrone**, R. O. Dendy, I. Furno, R. Sanchez, G. Zimbardo, A. Bovet, A. Fasoli, K. Gustafson, S. Perri, P. Ricci, F. Valentini, *Nonclassical transport and particle-field coupling: from laboratory plasmas to the solar wind*, **Space Science Reviews** 178, 233 (2013);
- **D. Perrone**, F. Valentini, S. Servidio, S. Dalena, P. Veltri, *Vlasov simulations of multi-ion plasma turbulence in the solar wind*, **The Astrophysical Journal**, 762, 99 (2013);
- **D. Perrone**, F. Valentini, P. Veltri, *The Role of Alpha Particles in the Evolution of the Solar-Wind Turbulence toward Short Spatial Scales*, **The Astrophysical Journal** 741, 43 (2011);
- **D. Perrone**, G. Nigro, P. Veltri, *A Shell Model Turbulent Dynamo*, **The Astrophysical Journal** 735, 73 (2011);
- F. Valentini, F. Califano, **D. Perrone**, F. Pegoraro, P. Veltri, *New ion-wave path in the energy cascade*, **Physical Review Letters** 106, 165002 (2011);
- **D. Perrone**, *A kinetic multi-component numerical model for the solar wind small-scale turbulence*, **Tesi di dottorato**, supervisor: Dr. F. Valentini, Prof. P. Veltri (2012)

Londra, 02/05/2018

Firma



MR F

**Tesi di dottorato:**

Titolo: "*Wigner Crystallization in polarizable and anisotropic systems*",  
University of L'Aquila, Italy.

Supervisors: Prof. S. Ciuchi (University of L'Aquila), Dr. S. Fratini (CNRS-Grenoble).

**Pubblicazioni:**

1- N. Hulea, S. Fratini, H. Xie, C. L. Mulder, N. N. Iossad, G. Rastelli, S. Ciuchi, A. F. Morpurgo,  
"*Tunable Fröhlich Polarons in Organic Single-Crystal Transistors*",  
Nature Materials 5, 982 (2006). [10.1038/nmat1774](https://doi.org/10.1038/nmat1774)

2- P. Stadler, W. Belzig, G. Rastelli,  
"*Ground-state cooling of a carbon nanomechanical resonator by spin-polarized current*",  
Phys. Rev. Lett. 113, 047201 (2014).  
<https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.113.047201>

3- G. Rastelli, I. M. Pop, F. W. J. Hekking,  
"*Quantum phase-slips in Josephson junction rings*",  
Phys. Rev. B 87, 174513 (2013).  
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4- T. Weissl, G. Rastelli, I. Matei, I. M. Pop, O. Buisson, F. W. J. Hekking, W. Guichard,  
"*Bloch band dynamics of a Josephson junction in an inductive environment*",  
Phys. Rev. B 91, 014507 (2015).  
<https://journals.aps.org/prb/abstract/10.1103/PhysRevB.91.014507>

5- Y. Vayrynen, G. Rastelli, W. Belzig, L. Glazman,  
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<https://journals.aps.org/prb/abstract/10.1103/PhysRevB.92.134508>

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"*Ground-State Cooling of a Mechanical Oscillator by Interference in Andreev Reflection*",  
Phys. Rev. Lett. 117, 197202 (2016).  
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7- G. Rastelli,  
"*Semi-classical formula for quantum tunneling in asymmetric double-well potentials*",  
Phys. Rev. A 86, 012106 (2012).  
<https://journals.aps.org/pra/abstract/10.1103/PhysRevA.86.012106>

8- G. Rastelli, M. Houzet, F. Pistolesi,  
"*Resonant magneto-conductance of a suspended carbon nanotube quantum dot*",  
EuroPhysics Letters 89, 57003 (2010).  
<http://iopscience.iop.org/article/10.1209/0295-5075/89/57003>

9- P. Stadler, W. Belzig, G. Rastelli  
"*Control of vibrational states by spin-polarized transport in a carbon nanotube resonator*",  
Phys. Rev. B 91, 085432 (2015).  
<https://journals.aps.org/prb/abstract/10.1103/PhysRevB.91.085432>

10- P.-J. Peters, F. Xu, K. Kaasbjerg, G. Rastelli, W. Belzig, R. Berndt,  
"Quantum coherent multi-electron processes in an atomic scale contact",  
Phys. Rev. Lett. 119, 066803 (2017).  
<https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.119.066803>

11- S. Gaudio, E. Cappelluti, G. Rastelli, L. Pietronero,  
"Finite-size Berezinskii-Kosterlitz-Thouless transition at grain boundaries in solid  $^4\text{He}$  and the role of  $^3\text{He}$  impurities",  
Phys. Rev. Lett. 101, 075301 (2008)  
<https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.101.075301>

12- D. Maile, S. Andergassen, W. Belzig, G. Rastelli,  
"Quantum phase transition with dissipative frustration",  
Phys. Rev. B 97, 155427 (2018).  
<https://journals.aps.org/prb/abstract/10.1103/PhysRevB.97.155427>

Konstanz, 01-05-2018

Giuseppa  
Rastelli

## Allegato 4 – Elenco delle pubblicazioni e della tesi di dottorato presentate datato e firmato (M.Sega)

(presentate ai fini della selezione)

1. P. Faccioli, M. Sega, F. Pederiva, and H. Orland, "Dominant pathways in protein folding", Phys. Rev. Lett., vol. 97, no. 10, p. 108101-1 (2006)
2. L. B. Pártay, P. Jedlovsky, M. Sega, "Molecular aggregates in aqueous solutions of bile acid salts. Molecular dynamics simulation study", J. Phys. Chem. B, vol. 111, no. 33, p. 9886 (2007)
3. M. Sega, P. Faccioli, F. Pederiva, G. Garberoglio, and H. Orland, "Quantitative protein dynamics from dominant folding pathways", Phys. Rev. Lett., vol. 99, no. 11, p. 118102-1 (2007)
4. M. Sega, R. Vallauri, and S. Melchionna, "Diffusion of water in confined geometry: The case of a multilamellar bilayer", Phys. Rev. E, vol. 72, no. 4, 1, p. 041201-1 (2005)
5. E. Autieri, M. Sega, F. Pederiva, and G. Guella, "Puckering free energy of pyranoses: A NMR and metadynamics-umbrella sampling investigation", J. Chem. Phys., vol. 133, no. 9, p. 095104-1 (2010)
6. I. Semenov, S. Raafatnia, M. Sega, V. Lobaskin, C. Holm, and F. Kremer, "Electrophoretic mobility and charge inversion of a colloidal particle studied by single-colloid electrophoresis and molecular dynamics simulations", Phys. Rev. E, vol. 87, no. 2, p. 022302-1 (2013)
7. J. Smiatek, M. Sega, C. Holm, U. D. Schiller, and F. Schmid, "Mesoscopic simulations of the counterion-induced electro-osmotic flow: A comparative study", J. Chem. Phys., vol. 130, no. 24, p. 244702-1 (2009)
8. S. Tyagi, M. Sützen, M. Sega, M. Barbosa, S. S. Kantorovich, C. Holm, "An iterative, fast, linear-scaling method for computing induced charges on arbitrary dielectric boundaries", J. Chem. Phys., vol. 132, no. 15, p. 154112-1 (2010)
9. M. Sega, S. S. Kantorovich, P. Jedlovsky, and M. Jorge, "The generalized identification of truly interfacial molecules (ITIM) algorithm for nonplanar interfaces", J. Chem. Phys., vol. 138, no. 4, p. 044110-1 (2013)
10. M. Sega, G. Horvai, and P. Jedlovsky, "Microscopic origin of the surface tension anomaly of water", Langmuir, vol. 30, p. 2969 (2014)



Allegato 4 – Elenco delle pubblicazioni e della tesi di dottorato presentate datate e firmate

11. M. Sega, E. Autieri and F. Pederiva, "On the calculation of puckering free energy surfaces", J. Chem. Phys., vol. 130, p. 225102-1 (2009)
12. M. Sega, M. Sbragaglia, L. Biferale and S. Succi "Regularization of the slip length divergence in water nanoflows by inhomogeneities at the Angstrom scale", Soft Matter, vol. 9, p. 8526 (2013)
13. Tesi di dottorato

Vienna, 19 aprile 2018,



## ELENCO DEI 12 PRODOTTI SCIENTIFICI SCELTI E DELLA TESI DI DOTTORATO

DICHIARAZIONE SOSTITUTIVA DI CERTIFICAZIONE  
AI SENSI DELL'ART. 46, D.P.R. 445/2000

DICHIARAZIONE SOSTITUTIVA DELL'ATTO DI NOTORIETA'  
AI SENSI DELL'ART. 47, D.P.R. 445/2000

Il sottoscritto Luca Fausto Tocchio

consapevole che chiunque rilascia dichiarazioni mendaci, forma atti falsi o ne fa uso è punito ai sensi del codice penale e delle leggi speciali in materia

DICHIARA

che le dodici pubblicazioni di seguito elencate e la tesi di dottorato, allegate alla domanda, sono conformi agli originali:

- 1) S. Karakuzu, L.F. Tocchio, S. Sorella, and F. Becca,  
"Superconductivity, charge-density waves, and antiferromagnetism in the Hubbard-Holstein model", Phys. Rev. B 96, 205145 (2017). DOI:10.1103/PhysRevB.96.205145. Date of publication: 27 November 2017.
- 2) R. Kaneko, L.F. Tocchio, R. Valentí, and F. Becca,  
"Charge orders in organic charge-transfer salts", New J. Phys. 19, 103033 (2017). DOI:10.1088/1367-2630/aa887b. Date of publication: 25 October 2017.
- 3) L.F. Tocchio, F. Becca, and S. Sorella,  
"Hidden Mott transition and large-U superconductivity in the two-dimensional Hubbard model", Phys. Rev. B 94, 195126 (2016). DOI:10.1103/PhysRevB.94.195126. Date of publication: 14 November 2016.
- 4) R. Kaneko, L.F. Tocchio, R. Valentí, F. Becca, and C. Gros,  
"Spontaneous symmetry breaking in correlated wave functions", Phys. Rev. B 93, 125127 (2016). DOI:10.1103/PhysRevB.93.125127. Date of publication: 17 March 2016.
- 5) J.P.F. LeBlanc et al. (Simons Collaboration on the Many-Electron Problem),  
"Solutions of the Two Dimensional Hubbard Model: Benchmarks and Results from a Wide Range of Numerical Algorithms", Phys. Rev. X 5, 041041 (2015). DOI: 10.1103/PhysRevX.5.041041. Date of publication: 14 December 2015.
- 6) L.F. Tocchio, C. Gros, X.-F. Zhang, and S. Eggert,  
"Phase diagram of the triangular extended Hubbard model", Phys. Rev. Lett. 113, 246405 (2014). DOI: 10.1103/PhysRevLett.113.246405. Date of publication: 12 December 2014.
- 7) A.C. Jacko, L.F. Tocchio, H.O. Jeschke, and R. Valentí,  
"Importance of anisotropy in the spin-liquid candidate  $\text{Me}_3\text{EtSb}[\text{Pd}(\text{dmit})_2]_2$ ", Phys. Rev. B 88, 155139 (2013). DOI: 10.1103/PhysRevB.88.155139. Date of publication: 31 October 2013.
- 8) L.F. Tocchio, H. Feldner, F. Becca, R. Valentí and C. Gros,  
"Spin-liquid versus spiral-order phases in the anisotropic triangular lattice", Phys. Rev. B 87, 035143 (2013). DOI: 10.1103/PhysRevB.87.035143. Date of publication: 31 January 2013.
- 9) L.F. Tocchio, F. Becca and C. Gros,  
"Strong renormalization of the Fermi-surface topology close to the Mott transition", Phys. Rev. B 86, 035102 (2012). DOI:10.1103/PhysRevB.86.035102. Date of publication: 5 July 2012.

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10) L.F. Tocchio, F. Becca and C. Gros,  
"Backflow correlations in the Hubbard model: An efficient tool for the study of the metal-insulator transition and the large-U limit", Phys. Rev. B 83, 195138 (2011). DOI: 10.1103/PhysRevB.83.195138. Date of publication: 31 May 2011.

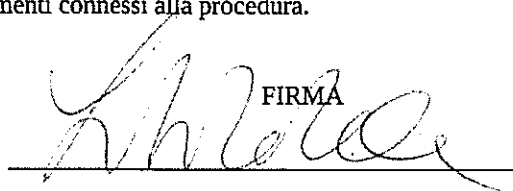
11) L.F. Tocchio, A. Parola, C. Gros and F. Becca,  
"Spin-liquid and magnetic phases in the anisotropic triangular lattice: The case of  $\kappa$ -(ET) $_2$ X", Phys. Rev. B 80, 064419 (2009). DOI: 10.1103/PhysRevB.80.064419. Date of publication: 26 August 2009.

12) L.F. Tocchio, F. Becca, A. Parola and S. Sorella,  
"Role of backflow correlations for the non-magnetic phase of the t-t' Hubbard model", Phys. Rev. B 78, 041101(R) (2008). DOI: 10.1103/PhysRevB.78.041101. Date of publication: 7 July 2008.

-) L.F. Tocchio,  
"A new variational wave function with backflow correlations for frustrated Hubbard models", Ph.D. thesis at SISSA. Supervisors: Prof. Sandro Sorella and Dr. Federico Becca. Date of defense: 24 October 2008.

Il sottoscritto, infine, esprime il proprio consenso affinché i dati personali forniti possano essere trattati, nel rispetto del D. Lgs. n.196/2003, per gli adempimenti connessi alla procedura.

Torino, 23/04/2018

 FIRMA

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## ELENCO PUBBLICAZIONI SELEZIONATE

### PhD Thesis:

Protein Internal Dynamics: Coarse-grained Investigation of the Structure-Function Relationship (2009).

### Pubblicazioni selezionate per la valutazione:

1. A. Zen, J.G. Brandenburg, J. Klimeš, A. Tkatchenko, D. Alfè, A. Michaelides.  
Fast and accurate quantum Monte Carlo for molecular crystals.  
Proc. Natl. Acad. Sci. U. S. A., 115: 1724-1729 (2018).  
IF: 9.661  
Times Cited: 0
2. M. Fitzner, L. Joly, M. Ma, G.C. Sosso, A. Zen, A. Michaelides.  
Communication: Truncated non-bonded potentials can yield unphysical behavior in molecular dynamics simulations of interfaces.  
J. Chem. Phys., 147: 121102 (2017).  
IF: 2.965  
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3. Y.S. Al-Hamdani, M. Rossi, D. Alfè, T. Tsatsoulis, B. Ramberger, J.G. Brandenburg, A. Zen, G. Kresse, A. Grüneis, A. Tkatchenko, A. Michaelides. Properties of the water to boron nitride interaction: From zero to two dimensions with benchmark accuracy. J. Chem. Phys., 147: 044710 (2017).  
IF: 2.965  
Times Cited: 1
4. J. Chen, A. Zen, J.G. Brandenburg, D. Alfè, A. Michaelides. Evidence for Stable Square Ice from Quantum Monte Carlo. Phys. Rev. B, in press (2016).  
IF: 3.836  
Times Cited: 7
5. A. Zen, L.M. Roch, S.J. Cox, X.L. Hu, S. Sorella, D. Alfè, A. Michaelides. Toward Accurate Adsorption Energetics on Clay Surfaces. J. Phys. Chem. C, 120: 26402-26413 (2016).  
IF: 4.563  
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6. A. Zen, S. Sorella, M.J. Gillan, A. Michaelides, D. Alfè.  
Boosting the accuracy and speed of quantum Monte Carlo: size consistency and time step.  
Phys. Rev. B, 93: 241118(R) (2016).  
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7. G.C. Sosso, J. Chen, S.J. Cox, M. Fitzner, P. Pedevilla, A. Zen, A. Michaelides.  
Crystal Nucleation in Liquids: Open Questions and Future Challenges in Molecular Dynamics Simulations.  
Chem. Rev., 116: 7078-7116 (2016).  
IF: 47.928  
Times Cited: 60
8. A. Zen, Y. Luo, G. Mazzola, L. Guidoni, S. Sorella.  
Ab-initio molecular dynamics simulation of liquid water by Quantum Monte Carlo.

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J. Chem. Phys., 142: 144111 (2015).

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9. A. Zen, E. Coccia, S. Gozem, M. Olivucci, L. Guidoni.

Quantum Monte Carlo Treatment of the Charge Transfer and Diradical Electronic Character in a Retinal Chromophore Minimal Model.

J. Chem. Theory Comput., 11: 992-1005 (2015).

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10. Y. Luo, A. Zen, S. Sorella.

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11. A. Zen, E. Coccia, Y. Luo, S. Sorella, L. Guidoni.

Static and dynamical correlation in diradical molecules by Quantum Monte Carlo using the Jastrow Antisymmetrized Geminal Power ansatz.

J. Chem. Theory Comput., 10: 1048-1061 (2014).

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12. A. Zen, Y. Luo, S. Sorella, L. Guidoni.

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J. Chem. Theory Comput., 9:4332-4350 (2013).

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Roma, 3 Maggio 2018

Andrea Zen

MR 5