

Group Publications

These are the most recent publications of the group (2006-2014). A complete list of the group's publications can be found following the links in the group members webpages.

[2014](#) [2013](#) [2012](#) [2011](#) [2010](#) [2009](#) [2008](#) [2007](#) [2006](#)

2014

- G. D'Adamo, A. Pelissetto and Carlo Pierleoni, "Accurate coarse-grained models for mixtures of colloids and linear polymers under good-solvent conditions", J. Chem. Phys. 141, 244905 (2014) DOI:10.1063/1.4904392
- J. Beutier, R. Vuilleumier, D. Borgis and S. Bonella, "Computing thermal Wigner densities with the phase integration method", J. Chem. Phys., 141, 084102 (2014) DOI: 10.1063/1.4892597
- G. D'Adamo, A. Pelissetto and Carlo Pierleoni, "Phase diagram of mixtures of colloids and polymers in the thermal crossover from Good to Theta solvent", J. Chem. Phys. 141, 024902 (2014) DOI:10.1063/1.4885818
- S. Bonella, D. Raimondo, E. Milanetti, A. Tramontano, G. Ciccotti, "Mapping the Hydropathy of Amino Acids Based on Their Local Solvation Structure", J. Phys. Chem. B, 118(24), 6604-6613 (2014) DOI:10.1021/jp500980x
- M. Micciarelli, S. Bonella et al., "Photophysics and Photochemistry of a DNA-Protein Cross-Linking Model: A Sinergistic Approach Combining Experiments and

Theory", J. Phys. Chem. B, 118(19), 4983-4992 (2014) DOI: 10.1021/jp4115018

- C. Violante, L. Chiodo, A. Mosca Conte, F. Bechstedt, O. Pulci, "Si(111) 2x1 surface isomers: DFT investigations on stability and doping effects", Surf. Sci. 621, 123-127 (2014) DOI: 10.1016/j.susc.2013.11.006

- S. Bonella, G. Ciccotti "Approximating Time-Dependent Quantum Statistical Properties", Entropy, 16(1), 86-109, (2014) DOI:10.3390/e16010086

- F. Gentile, M. Monteferrante, L. Chiodo, A. Toma, M. L. Coluccio, G. Ciccotti, E. Di Fabrizio, "Electroless formation of super-clusters of metal atoms: an experimental and numerical approach", Mol. Phys. 2014 (accepted) .

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2013

- P. Gargiani, S. Lisi, M. G. Betti, A. T. Ibrahimi, F. Bertran, P. Le Fèvre, L. Chiodo, "Orbital dependent Rashba splitting and electron-phonon coupling of 2D Bi phase on Cu (100) surface ", J. Chem. Phys. 139, 184707 (2013) DOI: 10.1063/1.4828865

- J. Beutier, M. Monteferrante, S. Bonella, R. Vuilleumier, G. Ciccotti "Gas phase infrared spectra via the phase integration quasi-classical method", Mol. Simulations., 40, 196-207, (2013) DOI: 10.1080/08927022.2013.843776

- F. Mouhat, S. Bonella, C. Pierleoni "Charge transport simulations of NaCl in an external magnetic field: the quest for the Hall effect", Mol. Phys. (2013) DOI: <http://dx.doi.org.10.1080/00268976.2013.846486>

- M. Monteferrante, S. Bonella, G. Ciccotti "Quantum dynamical structure factor of liquid neon via a quasiclassical symmetrized method", J. Chem. Phys. 138, 054118 (2013) DOI: 10.1063/1.4789760

- W. Rocchia, S. Bonella "A statistical mechanics handbook for protein-ligand binding simulation", Fronteers in bioscience 5, 478-495 (2013) PMID: 23277063

- G. Roma, L. Chiodo, "Selenium adsorption on Mo(110): a first principles investigation", Phys. Rev. B 87, 245420 (2013).

- A. Tanwar, E. Fabiano, P. E. Trevisanutto, L. Chiodo, F. Della Sala, "Accurate ionization potential of gold anionic clusters from density functional theory and many-body perturbation theory", Eur. Phys. J. B 86, 161 (2013) DOI: 10.1140/epjb/e2013-40016-5

- G. D'Adamo, A. Pelissetto and C. Pierleoni, "Predicting the thermodynamics by using state-dependent interactions", J. Chem. Phys. 138, 234107 (2013)
- G. D'Adamo, A. Pelissetto and C. Pierleoni, "Consistent coarse-graining strategy for polymer solutions in the thermal crossover from good to Theta solvent", J. Chem. Phys. 139, 34901 (2013)
- G. D'Adamo, A. Pelissetto and C. Pierleoni, "Depletion effects in colloid-polymer solutions", Mol. Phys., (2013) DOI:10.1080/00268976.2013.836255

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2012

- F. Sterpone, S. Bonella, S. Meloni "Early stage of the dehydrogenation of NaAlH₄ by ab initio rare events simulations", J. Phys. Chem. C, 19636-19643 (2012) DOI: 10.1021/jp3019588
- A. Poma, M. Monteferrante, S. Bonella, G. Ciccotti "The quantum free energy barrier for hydrogen vacancy diffusion in Na₃AlH₆", Phys. Chem. Chem. Phys., 14, 15458-15463 (2012) DOI: 10.1039/C2CP42536J
- G. D'Adamo, A. Pelissetto, C. Pierleoni "Consistent and transferable coarse-grained model for semidilute polymer solutions in good solvent", J. Chem. Phys. 137, 24901 (2012)
- G. D'Adamo, A. Pelissetto, C. Pierleoni "Polymers as compressible soft spheres", J. Chem. Phys. 136,224905 (2012).
- G. D'Adamo, A. Pelissetto, C. Pierleoni "Coarse-Graining strategies in polymer solutions", Soft Matter 8, 5151-5167 (2012)
- W. Babiacyk, S. Bonella, G. Ciccotti, M. L. Coluccio, F. Gentile and E. Di Fabrizio "Silver self aggregation in a nanodevice for enhanced Raman spectroscopy: experiments vs simplified modeling via molecular dynamics", Nanoscale, 4, 2362-2371 (2012), DOI: 10.1039/c2nr30145h
- G. Cottone, G. Lattanzi, G. Ciccotti and R. Elber "Multiphoton absorption of myoglobin-nitric oxide complex: relaxation by D-NEMD of a stationary state", J. Phys. Chem. B, (2012) DOI: 10.1021/jp21218x
- S. Bonella, S. Meloni and G. Ciccotti "Theory and methods for rare events", European Physical Journal B, 85, 97 (2012)

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- E. Liberatore, M.A. Morales, D.M. Ceperley, C. Pierleoni "Free-energy methods in Coupled Electron-Ion Monte Carlo", Mol. Phys. 109, 3029 (2011).

- M. Monteferrante, S. Bonella and G. Ciccotti "Linearized symmetrized quantum time correlation functions calculation via phase pre-averaging", Mol. Phys. 109, 3015-3027 (2011)
- S. Orlandini, S. Meloni and G. Ciccotti "Hydrodynamics from statistical mechanics: combined dynamical-NEMD and conditional sampling to relax an interface between two immiscible liquids", Phys. Chem. Chem. Phys. 13, 13177 (2011).
- M. Monteferrante, S. Bonella and G. Ciccotti "Short range hydrogen diffusion in Na₃AlH₆", Phys. Chem. Chem. Phys. 13, 10546 (2011).
- E. Liberatore, C. Pierleoni and D.M. Ceperley "Liquid-Solid transition in fully ionized hydrogen at ultra-high pressure", J. Chem. Phys. 134, 184505 (2011).
- G.Ciccotti, and S.Meloni "Temperature Accelerated Monte Carlo (TAMC): a method for sampling the free energy surface of non-analytical collective coordinates" CPPC, 13, 5952 (2011)
- F.Agostini, R.Vuilleumier, and G.Ciccotti "Infrared spectroscopy and effective modes analysis of the protonated water dimer H⁺ (H₂O)₂ at room temperature under H/D substitution" J.Chem.Phys., 134, 084302 (2011)
- F.Agostini, G.Ciccotti, and R.Vuilleumier "Infrared spectroscopy of small protonated water clusters at room temperature: an effective modes analysis", J.Chem.Phys., 134, 084303 (2011)

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2010

- G. D'Adamo, C. Pierleoni, "Crystalline free energy of micelles of diblock copolymer solutions", J. Chem. Phys., 133, 204902 (2010)
- W.I.Babiaczyk, S.Bonella, L.Guidoni, and G.Ciccotti "Hydration structure of the quaternary ammonium cations", J.Phys.Chem. B, 114, 15018-15028 (2010)
- S.Bonella, M.Monteferrante, C.Pierleoni, and G.Ciccotti "Path integral based calculations of symmetrized time correlation functions, I", J.Chem.Phys., 133, 164104 (2010)
- S.Bonella, M.Monteferrante, C.Pierleoni, and G.Ciccotti "Path integral based calculations of symmetrized time correlation functions, II", J.Chem.Phys., 133, 164105 (2010)
- A. Nassimi, S. Bonella, and R. Kapral, "Analysis of the quantum-classical Liouville equation in the mapping basis", J. Chem. Phys, 133, 134115-134126 (2010)
- P. Huo, S.Bonella, L. Chen, and D.F. Coker, "Linearization approximations for condensed phase non-adiabatic dynamics: multi-layered baths and brownian dynamics"

implementation"; Chem.Phys., 370, 87-97 (2010)

- L.Maragliano, G.Cottone, G.Ciccotti, and E.Vanden-Eijnden, "Mapping the network of pathways of CO diffusion in myoglobin"; JACS, 132, 1010 (2010)
- S.Bonella, G.Ciccotti, and R.Kapral, "Linearization approximations and Liouville quantum-classical dynamics"; Chem.Phys. Letts. 484, 4, 399-404 (2010)
- C.Hartmann, C.Schuetter, and G.Ciccotti, "On the linear response of mechanical systems with constraints"; J.Chem.Phys.,132, 111103 (2010)
- A.Jezierska, R.Vuilleumier, J.J.Panek, and G.Ciccotti, "Molecular properties investigations of an ortho- hydroxy Schiff base type compound: a combined DFT, AIM and first-principle molecular dynamics approach"; J.Phys.Chem.B, 114, 242-253 (2010)

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- M. L. Mugnai, S. Caprara, G. Ciccotti¹, C. Pierleoni, and M. Mareschal, "Formation of a compressible Rayleigh-Benard convective cell by dynamical non-equilibrium molecular dynamics"; J.Chem.Phys., 131, 064106, (2009)
- M.Monteferrante, S.Bonella, S.Meloni, and G.Ciccotti, "Modified single sweep method for reconstructing free energy landscapes"; Mol.Sim., 35, 1116-1129, (2009)
- M.Mareschal, S.Vantieghem, M.L.Mugnai, S.Caprara, G.Ciccotti, and C.Pierleoni, "Compressible convective instability by Molecular Dynamics"; in "Proceedings of Symposium on the 50th Anniversary of the Alder transition"; Y. Hiwatari & M. Isobe, Eds, Prog. of Theor.Phys. Suppl., 178, 15, (2009)
- C.Hartmann, C.Schuetter, G.Kalibaeva, M.Di Pierro, and G.Ciccotti, "Fast simulation of polymer chains"; J.Chem.Phys., 130, 144101 (2009)
- M.Venturoli, E.Vanden Eijnden, and G.Ciccotti, "Kinetics of phase transitions in the two-dimensional Ising models studied with the string method"; J.Math.Chem., 45, 188 (2009)
- S. Bonella, W. Rocchia, P. Amat, R. Nifosi and V. Tozzini, "SDPhound, a mutual information-based method to investigate specificity-determining positions"; Algorithms, 2, 764-789 (2009)

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2008

- E. Dunkel, S. Bonella, and D.F.Coker "Iterative linearized approach to non adiabatic dynamics", J. Chem. Phys., 129, 114106 (2008)
- P.L.Palla, C.Pierleoni, and G.Ciccotti, "Bulk viscosity of the Lennard-Jones system at the triple point by dynamical nonequilibrium molecular dynamics", Phys.Rev.E, 78, 021204 (2008)
- M.Monteferrante, S.Bonella, S.Meloni, E.Vanden Eijnden, and G.Ciccotti, "Calculations of free energy barriers for local mechanisms of hydrogen diffusion in alanates", Scientific Modeling & Simulation SMNS, vol. 15, 187 (2008)
- D.MacKernan, G.Ciccotti, and R.Kapral, "Trotter-Based Simulation of Quantum-Classical Dynamics", J.Phys.Chem., 112, 424-432, (2008)
- G.Ciccotti, E.Vanden-Eijnden, and T. Lelievre, "Projection of diffusions on submanifolds: Application to mean force computation", Comm.Pure and Applied Math., 61, 371-408,(2008)

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- F.Agostini, S.Caprara, and G.Ciccotti, "Do we have a consistent non adiabatic quantum-classical mechanics?", Europhys. Lett., 78, 30001, (2007)
- C.Simon, G.Ciccotti, and M.L.Klein, "Computing the acidity of liquids via ab initio molecular dynamics", Chem.Phys.Chem., 8, 2072, (2007)
- V.Marry, and G.Ciccotti, "Trotter derived algorithms for molecular dynamics with constraints : Velocity Verlet revisited", J.Comp.Phys., 222, 428, (2007)

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2006

- E.Vanden-Eijnden, and G.Ciccotti, "Second-order integrators for Langevin equations with holonomic constraints", Chem.Phys.Lett., 429, 310, (2006)
- M.S.Causo, G.Ciccotti, S.Bonella, and R.Vuilleumier, "An adiabatic linearized path integral approach for quantum time correlation functions II: A cumulant expansion method for improving convergence", J.Phys.Chem.B, 110, 3638, (2006)

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Book Chapters and Conference Proceedings

- L. Chiodo, A. Iacomino, M. Palumbo, A. Rubio, "Titania nanostructures electronic and optical response by high-level ab-initio computational approaches", in "Handbook of Functional Nanomaterials", Nova Science Publishers, Ltd. (New York – USA) (2013).
- G.Ciccotti, S.Caprara, and F.Agostini, "Do we have a consistent non-adiabatic quantum-classical statistical mechanics?" in: "Energy Transfer Dynamics in Biomaterial Systems", E.R.Bittner, I.Burghardt, V.May, and D.A.Micha, Eds. CPS, Springer, Berlin (2009)
- S.Bonella, D.F.Coker, D.Mac Kernan, R.Kapral, and G.Ciccotti, "Trajectory based

simulations of mixed quantum-classical systems” in: “Energy Transfer Dynamics in Biomaterial Systems”; E.R.Bittner, I.Burghardt, V.May, and D.A.Micha, Eds. CPS, Springer, Berlin (2009)

- D. F. Coker, L. Chen, P. Huo, and S. Bonella “Exploring the linearized approximation for condensed phase non-adiabatic dynamics: multi-layered baths”, Multidimensional Quantum Mechanics with trajectories, editors Dmitry Shalashilin and Marcelo Miranda, CCP6 (2009)

- M.Mareschal, S.Vantighem, M.L.Mugnai, S.Caprara, G.Ciccotti, and C.Pierleoni, “Compressible convective instability by Molecular Dynamics” Y.Hiwatari & M.Isobe, Eds Prog. of Theor.Phys.Suppl., 178, 15 (2009)

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