List of Publications by Giovanni Ciccotti

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2021

227) DD.Girardier, A.Coretti, G.Ciccotti, and S.Bonella
"Mass-Zero constrained dynamics and statistics for the shell model in magnetic field"
European Physical Journal B, 94, e158, (2021)

226) D.Macuglia, B.Roux, and G.Ciccotti
"The breakthrough of a quantum chemist by classical dynamics: Martin Karplus and the birth of computer simulations of chemical reactions"
European Physical Journal H, 46, ? , (2021)

225) C.Templeton, R.Elber, M.Ferrario, and G.Ciccotti
"A new boundary driven NEMD scheme for heat and particle diffusion in binary mixtures"
Molecular Physics, ? , e1892849, (2021)

224) G.Ciccotti, and L.Rondoni
"Jarzynski on work and free energy relations: The case of variable volume"
AICHE Journal 67, e17082, (2021)

2020

223) F.Talotta, F.Agostini, and G.Ciccotti
"Quantum Trajectories for the Dynamics in the Exact Factorization Framework: A Proof-of-Principle Test"
Journal of Physical Chemistry A, 124, 6764, (2020)

222) A.Coretti, L.Scalfi, C.Bacon, B.Rotenberg, R.Vuilleumier, G.Ciccotti, M.Salanne, and S.Bonella
"Mass-zero constrained molecular dynamics for electrode charges in simulations of electrochemical systems"
J.Chem.Phys. 152, 194701, (2020)

221) D.Macuglia, B.Roux, and G.Ciccotti
"Sense Experiences and "Necessary Simulations": Four Centuries of Scientific Change from Galileo to Fundamental Computer Simulations"
KNOW: A Journal on the Formation of Knowledge 4, 63-87, (2020)

220) S.Bonella, A.Coretti, R.Vuilleumier, and G.Ciccotti
"Adiabatic motion and statistical mechanics via mass zero constrained dynamics"
PCCP, 22, 10775-10785, (2020)

2019

219) ASF.Oliveira, CJ.Edsall, CJ.Woods, P.Bates, G.Viedma Nunez, S.Wonnacott, I.Bermudez, G.Ciccotti, T.Gallagher, RB.Sessions, and AJ.Mulholland
"A general mechanism for signal propagation in the nicotinic acetylcholine receptor family"
JACS, 141, 19953-19958, (2019)

218) G.Gobbo, G.Ciccotti, and BL.Trout
"On computing the solubility of molecular systems subject to constraints using the extended Einstein crystal method"
J.Chem.Phys. 150 (20), 201104, (2019)

217) MA.Bellucci, G.Gobbo, TK.Wijethunga, G.Ciccotti, and BL.Trout
"Solubility of paracetamol in ethanol by molecular dynamics using the extended Einstein crystal method and experiments"
J.Chem.Phys. 150, 094107, (2019)

216) M.Lauricella, L.Chiodo, G.Ciccotti, and A.Albinati
"Ab initio accelerated molecular dynamics study of the hydride ligands in the ruthenium complex: Ru (H 2) 2 H 2 (P (C 5 H 9) 3) 2"
PCCP 21, 25247-25257, (2019)

215) G.Ciccotti, and L.Delle Site
"The physics of open systems for the simulation of complex molecular environments in soft matter"
Soft Matter 15, 2114-2124, (2019)

2018

214) A.Coretti, S.Bonella, and G.Ciccotti
"Communication: Constrained molecular dynamics for polarizable models"
J.Chem.Phys. 149, 191102, (2018)

213) A.Coretti, S.Bonella, L.Rondoni, and G.Ciccotti
"Time reversal and symmetries of time correlation functions"
Mol.Phys. 116, 3097-3103, (2018)

212) G.Battimelli, and G.Ciccotti
"Berni Alder and the pioneering times of molecular simulation"
EPJ H 43, 303-335, (2018)

211) F.Agostini, I.Tavernelli, and G.Ciccotti
"Nuclear quantum effects in electronic (non) adiabatic dynamics"
EPJ B 91, 139, (2018)

210) G.Ciccotti, M.Ferrario, and C.Schütte
"Molecular Dynamics vs. Stochastic Processes: Are We Heading Anywhere?"
Entropy 20, 348, (2018)

209) A.Perilli, C.Pierleoni, G.Ciccotti, and JP.Ryckaert
"On the force–velocity relationship of a bundle of rigid bio-filaments"
J.Chem.Phys. 148, 095101, (2018)

208) G.Ciccotti, and M.Ferrario
"Holonomic Constraints: A Case for Statistical Mechanics of Non-Hamiltonian Systems"
Computation 6, 11, (2018)

207) G.Gobbo, MA.Bellucci, GA.Tribello, G.Ciccotti, and BL.Trout
"Nucleation of molecular crystals driven by relative information entropy"
J.Chem.Th.Comp. 14, 959-972, (2018)

2017

206) M.Lauricella, G.Ciccotti, NJ.English, B.Peters, and S.Meloni
"Mechanisms and nucleation rate of methane hydrate by dynamical nonequilibrium molecular dynamics"
J.Phys.Chem. C 121, 24223-24234, (2017)

205) S.Bonella, M.Ferrario, and G.Ciccotti
"Thermal diffusion in binary mixtures: Transient behavior and transport coefficients from equilibrium and nonequilibrium molecular dynamics"
Langmuir 33, 11281-1129, (2017)

204) L.Delle Site, G.Ciccotti, and C.Hartmann
"Partitioning a macroscopic system into independent subsystems"
J.Stat.Mech. Theory and Experiment 2017, 083201, (2017)

203) S.Bonella, A.Coretti, L.Rondoni, and G.Ciccotti
"Time-reversal symmetry for systems in a constant external magnetic field"
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202) P.Koltai, G.Ciccotti, and C.Schuette
"On metastability and Markov state models for non-stationary molecular dynamics"
J.Chem.Phys., 145, 174103, (2016)

201) M.Ferrario, S.Bonella, and G.Ciccotti
"On the establishment of thermal diffusion in binary Lennard-Jones liquids"
EPJ-Special Topics, 225, 1629-1642, (2016)

200) T.A.Hunt, S.Mogurampelly, G.Ciccotti, C.Pierleoni, and J.P.Ryckaert
"Particle-based modeling of living actin filaments in an optical trap"
Polymers, 8, 343, (2016)

199) A.Perilli, C.Pierleoni, G.Ciccotti, and J.P.Ryckaert
"On the properties of a bundle of flexible actin filaments in an optical trap"

J.Chem.Phys., 144, 245102, (2016)

198) G.Ciccotti, S.Bonella, M.Ferrario, and C.Pierleoni
"Probabilistic derivation of spatiotemporal correlation functions in the hydrodynamic limit"
J.Phys.Chem.B, 120, 1996-2000, (2016)

197) R.E.Breier, R.L.B.Selinger, G.Ciccotti, S.Herminghaus, and M.G.Mazza
"Spontaneous chiral symmetry breaking in collective active motion"
Phys.Rev.E, 93, 022410, (2016)

196) G.Ciccotti, and M.Ferrario
"Non-equilibrium by molecular dynamics: a dynamical approach"
Mol.Sim., 42, 1385-1400, (2016)

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195) C.Pierleoni, G.Ciccotti, and J.P.Ryckaert
"A semi-flexible model prediction for the polymerization force exerted by a living F-actin filament on a fixed wall"
J.Chem.Phys., 143, 145101, (2015)

194) J.Beutier, R.Vuilleumier, S.Bonella, and G.Ciccotti
"Gas phase infrared spectra from quasi-classical Kubo time correlation functions"
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193) S.Bonella, and G.Ciccotti
"An introduction to the problem of bridging quantum and classical dynamics"
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192) S.Meloni, and G.Ciccotti
"*Free energies for rare events: temperature accelerated MD and MC"*
EPJ-Special Topics, 224, 2389-2407, (2015)

191) G.Ciccotti, and E.Vanden-Eijnden
"The trees and the forest"
EPJ-Special Topics, 224, 2515-2518, (2015)

190) F.Agostini, G.Ciccotti, A.Savin, and R.Vuilleumier
"Maximum probability domains for the analysis of the microscopic structure of liquids"
J.Chem.Phys., 142, 064117, (2015)

189) L.Chiodo, T.Malliavin, L.Maragliano, G.Cottone, and G.Ciccotti
"A structural model of the human alpha 7 nicotinic receptor in an open conformation"
PLOS ONE, 10, e0133011, (2015)
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188) M.Lauricella, S.Meloni, S.Liang, NJ.English, PG.Kusalik, and G.Ciccotti
"Clathrate structure-type recognition: application to hydrate nucleation and crystallisation"
J.Chem.Phys., 142, 244503, (2015)

DOI: 10.1063/1.4922696

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187) S.Bonella, G.Ciccotti, and L.Rondoni
"Time reversal symmetry in time-dependent correlation functions for systems in a magnetic field"
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DOI: 10.1209/0295-5075/108/60004

186) M.Pourali, S.Meloni, F.Magaletti, A.Maghari, C.M.Casciola, and G.Ciccotti
"Relaxation of a steep density gradient in a simple fluid: comparison between atomistic and continuum modeling"
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"Methane clathrate hydrate nucleation mechanism by advanced molecular simulations"
J.Phys.Chem.C, 118, 22847-22857 (2014)
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"Temperature-accelerated molecular dynamics gives insights into globular conformations sampled in the free state of the AC catalytic domain"
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DOI: 10.1002/prot.24612

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"Exploring the conformational dynamics of alanine dipeptide in solution subjected to an external electric field: a nonequilibrium molecular dynamics simulation"
JCTC, 10, 1376-1386 (2014)
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178) S.Bonella, and G.Ciccotti
"Approximating time-dependent quantum statistical properties"
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177) J.Beutier, S.Bonella, R.Vuilleumier, and G.Ciccotti
"Gas phase infrared spectra via the phase integration quasi-classical method"
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175) J.Lucid, S.Meloni, D.Mac Kernan, E.Spohr, and G.Ciccotti
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170) W.I.Babiaczyk, S.Bonella, G.Ciccotti, M.L.Coluccio, F.Gentile, and E.Di Fabrizio
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"Multiphoton absorption of myoglobin nitric oxide complex: relaxation by D-NEMD of a stationary state"
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166-B) C.Hartmann, J.C.Latorre, and G.Ciccotti
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"Short range hydrogen diffusion in Na_3AlH_6"
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154) S.Bonella, M.Monteferrante, C.Pierleoni, and G.Ciccotti
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153) L.Maragliano, G.Cottone, G.Ciccotti, and E.Vanden-Eijnden
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152) C.Hartmann, C.Schuette, and G.Ciccotti
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145-B) G.Ciccotti, S.Caprara, and F.Agostini
"Do we have a consistent non-adiabatic quantum-classical statistical mechanics?"
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