

List of Publications by Giovanni Ciccotti

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2017

203) S.Bonella, A.Coretti, L.Rondoni, and G.Ciccotti
“Time-reversal symmetry for systems in a constant external magnetic field”
Phys.Rev.E, Submitted (2017)

2016

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)

2015

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”

Mol.Phys., 113, 2894-2904, (2015)

193) S.Bonella, and G.Ciccotti

“An introduction to the problem of bridging quantum and classical dynamics”

EPJ-Special Topics, 224, 2305-2320, (2015)

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)

DOI: 10.1371/journal.pone.013301

188) M.Lauricella, S.Meloni, S.Liang, N.J.English, P.G.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

2014

187) S.Bonella, G.Ciccotti, and L.Rondoni

“Time reversal symmetry in time-dependent correlation functions for systems in a magnetic field”

EPL, 108, 60004 (2014)

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”

J.Chem.Phys., 141, 154107 (2014)

DOI: 10.1063/1.4897977

185) M.Lauricella, S.Meloni, N.English, P.Barons, and G.Ciccotti

“Methane clathrate hydrate nucleation mechanism by advanced molecular simulations”

J.Phys.Chem.C, 118, 22847-22857 (2014)

DOI: 10.1021/jp5052479

184) E.Selva, T.Huynh, G.Ciccotti, L.Maragliano, and T.E.Malliavin
“Temperature-accelerated molecular dynamics gives insights into globular conformations sampled in the free state of the AC catalytic domain”
Proteins, 82, 2483-2496 (2014)
DOI: 10.1002/prot.24612

183) H.Wang, C.Schuetter, G.Ciccotti, and L.Delle Site,
“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)
DOI: 10.1021/ct400993e

182) S.Bonella, D.Raimondo, E.Milanetti, A.Tramontano, and G.Ciccotti
“Mapping the hydrophathy of amino acids based on their local solvation structure”
J.Phys.Chem.B, 118, 6604-6613 (2014)
DOI: 10.1021/jp500980x

181) F.Gentile, M.Monteferrante, L.Chiodo, A.Toma, M.L.Coluccio, G.Ciccotti, and E.Di Fabrizio
“Electroless formation of silver nanoaggregates: an experimental and molecular dynamics approach”
Mol.Phys., 112, 1375-1388 (2014)
DOI: 10.1080/00268976.2014.902518

180) Z.Mohammad Hosseini Naveh, T.E.Malliavin, L.Maragliano, G.Cottone, and G.Ciccotti
“Conformational changes in acetylcholine binding protein investigated by temperature accelerated molecular dynamics”
PLOS ONE, 9, e88555 (2014)
DOI: 10.1371/journal.pone.0088555

179) G.Ciccotti, and M.Ferrario
“Dynamical non-equilibrium molecular dynamics”
Entropy, 16, 233-257 (2014)
DOI: 10.3390/e16010233

178) S.Bonella, and G.Ciccotti
“Approximating time-dependent quantum statistical properties”
Entropy, 16, 86-109 (2014)
DOI:10.3390/e16010086

177) J.Beutier, S.Bonella, R.Vuilleumier, and G.Ciccotti
“Gas phase infrared spectra via the phase integration quasi-classical method”
Mol.Sim., 40, 196-207 (2014)
DOI: 10.1080/08927022.2013.843776

2013

176) M.Monteferrante, S.Bonella, and 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

175) J.Lucid, S.Meloni, D.Mac Kernan, E.Spohr, and G.Ciccotti
“Probing the structures of hydrated nafion in different morphologies using temperature-accelerated molecular dynamics simulations”
J.Chem.Phys. 117, 774-782 (2013)
DOI: 10.1021/jp309038n

174) P.A.Geslin, G.Ciccotti, and S.Meloni
“An observable for vacancy characterisation and diffusion in crystals”
J.Chem.Phys. 138, 144103 (2013)
DOI: 10.1063/1.4796322

173) A.Elena, S.Meloni, and G.Ciccotti
“Equilibrium and rate constants, and reaction mechanism of the HF dissociation in the HF(H₂O)₇ cluster by ab initio rare event simulations”
J.Phys.Chem. A, 117, 13039-13050 (2013)
DOI: dx.doi.org/10.1021/jp406982h

2012

172) A.Poma, M.Monteferrante, S.Bonella, and G.Ciccotti
“The quantum free energy barrier for hydrogen vacancy diffusion in Na₃AlH₆”
PCCP, 14, 15458-15463 (2012)
DOI: 10.1039/c2cp42536j1

171) S.Bonella, S.Meloni, and G.Ciccotti
“Theory and methods for rare events”
EPJ B, 85, 97 (2012)
DOI: 10.1140/epjb/e2012-20366-2

170) W.I.Babiaczyk, 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

169) 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, 116, 3397-3410 (2012)
DOI: 10.1021/jp212148x

168) S.Fritsch, S.Poblete, C.Junghans, G.Ciccotti, L.Delle Site, and K.Kremer
“Adaptive resolution molecular dynamics simulation through coupling to an internal particle reservoir”

2011

167) M.Monteferrante, S.Bonella, and G.Ciccotti
“*Linearized symmetrized quantum time correlation functions calculation via phase preaveraging*”
Mol.Phys., 109, 3015-3027 (2011)

166-B) C.Hartmann, J.C.Latorre, and G.Ciccotti
“*On two possible definitions of the free energy for collective variables*”
EPJ-Special Topics, 200, 73-89 (2011)

165-B) P.Español, J.A.de la Torre, M.Ferrario, and G.Ciccotti
“*Coarse-graining stiff bonds*”
EPJ-Special Topics, 200, 107-129 (2011)

164-B) S.Orlandini, S.Meloni, and G.Ciccotti
“*Hydrodynamics from dynamical non-equilibrium MD*”
In: “***Non-Equilibrium Statistical Physics Today - Proceedings of the 11th Granada Seminar on Computational and Statistical Physics***”
P.L.Garrido, J.Marro, and F.de los Santos, Eds.
AIP, Conferences Proceedings 1332, Melville, New York, 2011

163) S.Meloni, S.Orlandini, and G.Ciccotti
“*Combining rare events techniques: phase change in Si nanoparticles*”
J.Stat.Phys., 145, 812-830 (2011)

162) 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*”
PCCP, 13, 13177 (2011)

161) M.Monteferrante, S.Bonella, and G.Ciccotti
“*Short range hydrogen diffusion in Na₃AlH₆*”
PCCP, 13, 10546 (2011)

160) 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)

159) 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)

158) 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)

157) A.Jezierska-Mazzarello, J.Panek, R.Vuilleumier, A.Koll, and G.Ciccotti
“Direct observation of the substitution effects on the hydrogen bridge dynamics in selected Schiff bases - A comparative molecular dynamics study”
J.Chem.Phys., 134, 034308 (2011)

2010

156) 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)

155) 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)

154) 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)

153) L.Maragliano, G.Cottone, G.Ciccotti, and E.Vanden-Eijnden
“Mapping the network of pathways of CO diffusion in mioglobin”
JACS, 132, 1010-1017 (2010)

152) C.Hartmann, C.Schuetz, and G.Ciccotti
“On the linear response of mechanical systems with constraints”
J.Chem.Phys., 132, 111103 (2010)

151) 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)

2009

150) S.Bonella, G.Ciccotti, and R.Kapral
“Linearization approximations and Liouville quantum-classical dynamics”
Chem.Phys.Lett., 484, 399-404 (2009)

149) M.L.Mugnai, S.Caprara, G.Ciccotti, C.Pierleoni, and M.Mareschal
“Transient hydrodynamical behavior by dynamical nonequilibrium molecular dynamics: The formation of convective cells”
J.Chem.Phys., 131, 064106 (2009)

148) M.Monteferrante, S.Bonella, S.Meloni, and G.Ciccotti
“Modified single sweep method for reconstructing free energy landscapes”

Mol.Sim., 35, 1116-1129 (2009)

147) M.Mareschal, S.Vantighem, 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 and M.Isobe, Eds

Prog. of Theor.Phys.Suppl., 178, 15 (2009)

146-B) 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

145-B) 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

144) C.Hartmann, C.Schuetter, G.Kalibaeva, M.Di Pierro, and G.Ciccotti

“Fast simulation of polymer chains”

J.Chem.Phys., 130, 144101 (2009)

143) M.Venturoli, E.Vanden Eijnden, and G.Ciccotti

“Kinetics of phase transitions in the two-dimensional Ising models studied with the string methods”

J.Math.Chem., 45, 188 (2009)

2008

142) 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)

141) E.Vanden Eijnden, M.Venturoli, G.Ciccotti, and R.Elber

“On the assumptions underlying milestoning”

J.Chem.Phys., 129, 174102 (2008)

140) 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”

Scient.Model. and Simul. SMNS, 15, 187 (2008)

139) D.Mac Kernan, G.Ciccotti, and R.Kapral

“Trotter-Based Simulation of Quantum-Classical Dynamics”

J.Phys.Chem., 112, 424 (2008)

138) 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 (2008)

2007

137) F.Agostini, S.Caprara, and G.Ciccotti
“*Do we have a consistent non adiabatic quantum-classical mechanics?*”
Europhys.Lett., 78, 30001 (2007)

136) C.Simon, G.Ciccotti, and M.L.Klein
“*Computing the acidity of liquids via ab initio molecular dynamics*”
Chem.Phys.Chem., 8, 2072 (2007)

135) V.Marry, and G.Ciccotti
“*Trotter derived algorithms for molecular dynamics with constraints: Velocity Verlet revisited*”
J.Comp.Phys., 222, 428 (2007)

2006

134) E.Vanden Eijnden, and G.Ciccotti
“*Second-order integrators for Langevin equations with holonomic constraints*”
Chem.Phys.Lett., 429, 310 (2006)

133) 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)

132) L.Maragliano, A.Fischer, E.Vanden Eijnden, and G.Ciccotti
“*String method in collective variables: minimum free energy paths and isocommittor surfaces*”
J.Chem.Phys., 125, 024106 (2006)

131-B) R.Kapral, and G.Ciccotti
“*Transport Coefficients of Quantum-Classical Systems*”
In: “**Computer Simulations in Condensed Matter: From Materials to Chemical Biology**”
M.Ferrario, G.Ciccotti, and K.Binder, Eds.
LNP, Springer, Berlin, 2006

130-B) G.Ciccotti, D.Coker, and R.Kapral
“*Quantum statistical dynamics with trajectories*”
In: “**Quantum Dynamics of Complex Molecular Systems**”
I.Burghardt, and D.Micha, Eds.
CPS, Springer, Berlin, 2006

129) G.Kalibaeva, R.Vuilleumier, S.Meloni, A.Alavi, G.Ciccotti, and R.Rosei
“*Ab initio simulation of carbon clustering on Ni(111) surface: a model of the poisoning of nickel based catalysts*”

J.Phys.Chem.B, 110, 3638 (2006)

128) F.Pizzitutti, A.Giansanti, P.Ballario, P.Ornaghi, P.Torreri, G.Ciccotti., and P.Filetici
“*Relevant role of loop ZA and Pro371 in the function of yeast Gcn5p bromodomain: evidences from Molecular Dynamics and experiments*”
Journal of Molecular Recognition, 19, 1 (2006)

2005

127) G.Ciccotti, R.Kapral, and E.Vanden Eijnden
“*Blue Moon sampling, vectorial reaction coordinates, and unbiased constrained dynamics*”
Chem.Phys.Chem., 6, 1809 (2005)

126) G.Costantini, U.Marini Bettolo Marconi, G.Kalibaeva, and G.Ciccotti
“*The inelastic hard dimer gas: a non spherical model for granular matter*”
J.Chem.Phys., 122, 164505 (2005)

125) M.S.Causo, G.Ciccotti, D.Montemayor, S.Bonella, and D.F.Coker
“*An adiabatic linearized path integral approach for quantum time correlation functions: Electronic transport in metal-molten salt solutions*”
J.Phys.Chem.B, 109, 6855 (2005)

124-B) G.Ciccotti, R.Kapral
“*Molecular Dynamics: An account of its evolution*”
In: “***Theory and Applications of Computational Chemistry: The First Forty Years***”
C.Dykstra, G.Frenking, K.Kim, G.Scuseria, Eds.
Elsevier, Amsterdam, 2005

123-B) G.Ciccotti, R.Kapral, and A.Sergi
“*Nonequilibrium Molecular Dynamics*”
In: “***Encyclopedia of Materials Modeling***”
S.Yip, Ed.
Springer, New York, 2005

122-B) G.Ciccotti, R.Kapral, and A.Sergi
“*Simulating reactions that occur once in a blue moon*”
In: “***Encyclopedia of Materials Modeling***”
S.Yip, Ed.
Springer, New York, 2005

121) G.Cottone, S.Giuffrida, G.Ciccotti, and L.Cordone
“*Structure-dynamics coupling between protein and external matrix in sucrose coated and in trehalose coated Mb-Co. II. A simulative study*”
Biophys.J., 59, 291 (2005)

2004 - 2000

120-P) L.Maragliano, M.Ferrario, and G.Ciccotti

- “Effective binding force calculation in dimeric proteins”
Molecular Simulations, 30, 807 (2004)
- 119-P) G.Ciccotti, and M.Ferrario
“Blue Moon approach to rare events”
Molecular Simulations, 30, 787 (2004)
- 118) R.L.C.Akkermans, and G.Ciccotti
“On the equivalence of atomic and molecular pressure”
J.Phys.Chem.B, 108, 6866 (2004)
- 117-P) G.Ciccotti, and G.Kalibaeva
“Deterministic and stochastic algorithms for mechanical systems under constraints”
Phil.Trans. of the Royal Soc., 362, 1583 (2004)
- 116-B) G.Ciccotti, and G.Kalibaeva
“Molecular dynamics of complex systems: non-hamiltonian, constrained, quantum-classical”
In: “**Novel Methods in Soft Matter Simulations**”
M.Kartunnen, Ed.
Lecture Notes in Physics, Vol.640, p.150
Springer, Berlin, 2004
- 115) L.Maragliano, G.Cottone, L.Cordone, and G.Ciccotti
“Atomic mean square displacements in proteins by Molecular Dynamics: a case for analysis of variance”
Biophys.J., 86, 2765 (2004)
- 114) G.Kalibaeva, and G.Ciccotti
“Simulation of a diatomic liquid using hard spheres model”
J.Stat.Phys, 115, 701 (2004)
- 113) I.Coluzza, M.Sprik, and G.Ciccotti
“Constrained reaction coordinate dynamics for systems with constraints”
Mol.Phys., 101, 2885 (2003)
- 112) A.Ricci, and G.Ciccotti
“Algorithms for brownian dynamics”
Mol.Phys., 101, 1927 (2003)
- 111) G.B.Suffritti, P.Demontis, and G.Ciccotti
“Comment on: Does lattice vibration drive diffusion in zeolites?”
J.Chem.Phys., 118, 3439 (2003)
- 110) A.Sergi, D.Mac Kernan, G.Ciccotti, and R.Kapral
“Simulating quantum dynamics in classical environments”
Theor.Chem.Accounts, 110, 49 (2003)
- 109-P) R.Kapral, and G.Ciccotti
“A statistical mechanical theory of quantum dynamics in classical environments”

In: ***“Bridging time scales: Molecular simulations for the next decade”***

SIMU Conference, Konstanz 2001

P.Nielaba, M.Mareschal, and G.Ciccotti, Eds.

Springer, Berlin, 2003

108) G.Kalibaeva, M.Ferrario, and G.Ciccotti

“Constant pressure-constant temperature molecular dynamics: a correct constrained NPT ensemble using the molecular virial”

Mol.Phys., 101, 765 (2003)

107) D.Mac Kernan, R.Kapral, and G.Ciccotti

“Sequential short-time propagation of quantum-classical dynamics”

J.Phys.: Condens. Matter, 14, 9069 (2002)

106) A.Perronace, G.Ciccotti, F.Leroy, A.H.Fuchs, and B.Rousseau

“Soret coefficient for liquid Argon-Krypton mixtures via equilibrium and non-equilibrium Molecular Dynamics: a comparison with experiments”

Phys.Rev.E, 66, 031201 (2002)

105) M.Ferrario, G.Ciccotti, E.Spohr, T.Cartailier, and P.Turq

“Solubility of KF in water by Molecular Dynamics using the Kirkwood integration method”

J.Chem.Phys., 117, 4947 (2002)

104) G.Cottone, L.Cordone, and G.Ciccotti

“Protein-trehalose-water structures in trehalose coated carboxy-myoglobin”

J.Chem.Phys., 117, 9862 (2002)

103) D.Mac Kernan, G.Ciccotti, and R.Kapral

“Surface-hopping dynamics of a spin-boson system”

J.Chem.Phys., 116, 2346 (2002)

102) A.Sergi, G.Ciccotti, M.Falconi, A.Desideri, and M.Ferrario

“Effective binding force calculation in a dimeric protein by molecular dynamics simulation”

J.Chem.Phys., 116, 6329 (2002)

101) T.O.White, G.Ciccotti, and J.P.Hansen

“Brownian dynamics with constraints”

Mol.Phys., 99, 2023 (2001)

100) S.Nielsen, R.Kapral, and G.Ciccotti

“Statistical mechanics of quantum-classical systems”

J.Chem.Phys., 115, 5805 (2001)

99) A.Perronace, J.M.Simon, B.Rousseau, and G.Ciccotti

“Flux expressions and nonequilibrium molecular dynamics perturbations for models of semiflexible molecules”

Mol.Phys., 99, 1139 (2001)

98) G.Ciccotti, G.J.Martyna, S.Melchionna, and M.E.Tuckerman

“Constrained isothermal-isobaric molecular dynamics with full atomic virial”
J.Phys.Chem.B, 105, 6710 (2001)

97) M.E.Tuckerman, G.Ciccotti, and G.J.Martyna
“Non-hamiltonian molecular dynamics: generalizing hamiltonian phase space principles to non-hamiltonian systems”
J.Chem.Phys., 115, 1678 (2001)

96) G.Cottone, L.Cordone, and G.Ciccotti
“MD simulation of carboxy-myoglobin embedded in a thehalose-water matrix”
Biophys.J., 80, 931 (2001)

95) G.Ciccotti, and M.Ferrario
“Rare events by constrained molecular dynamics”
J.Mol.Liquids, 89, 1 (2000)

94) S.Nielsen, R.Kapral, and G.Ciccotti
“Non-adiabatic dynamics in mixed quantum-classical systems”
J.Stat.Phys., 101, 225 (2000)

93) S.Nielsen, R.Kapral, and G.Ciccotti
“Mixed quantum-classical Surface hopping dynamics”
J.Chem.Phys., 112, 6543 (2000)

92) S.Fioravanti, R.G.Winkler, G.Ciccotti, C.Margheritis, and M.Villa
“Hydration of beta-cyclodextrin. An MD Study”
J.Comp.Aided Mol.Design, 14, 659 (2000)

1999 - 1995

91) R.Kapral, and G.Ciccotti
“Mixed quantum-classical dynamics”
J.Chem.Phys., 110, 8919 (1999)

90) G.Ciccotti, C.Pierleoni, F.Capuani, and V.S.Filinov
“Wigner approach to the semiclassical dynamics of a quantum many-body system: the dynamic scattering function of ^4He ”
Comp.Phys.Comm., 121-122, 452 (1999)

89) M.Sprik, and G.Ciccotti
“Free energy from constrained molecular dynamics”
J.Chem.Phys., 109, 7737 (1998)

88) M.Falconi, A.Desideri, A.Cupane, M.Leone, G.Ciccotti, A.Gambacurta, F.Ascoli
*“Structural dynamics properties of the Thr72--> Ile mutant of the homodimeric haemoglobin from *Scapharca inaequalvis*. A Molecular Dynamics simulation and Low Temperature Optical Spectroscopy study”*
Biophys.J., 75, 2489 (1998)

- 87) A.Palma, A.Pasquarello, G.Ciccotti, and R.Car
"Cu⁺⁺ and Li⁺⁺ interaction with Polyethylene oxide by ab-initio Molecular Dynamics"
 J.Chem.Phys., 108, 9933 (1998)
- 86-B) D.Laria, G.Ciccotti, D.F.Coker, M.Ferrario, and R.Kapral
"Nonadiabatic Molecular Dynamics methods for diffusion"
 In: **"Simulation of classical and quantum dynamics in condensed phase"**
 Euroconference 1997, B.J.Berne, G.Ciccotti, and D.F.Coker, Eds.
 World Scientific, Singapore, 1998
- 85-B) G.Ciccotti, and M.Ferrario
"Constrained and Nonequilibrium Molecular Dynamics"
 In: **"Simulation of classical and quantum dynamics in condensed phase"**
 Euroconference 1997, B.J.Berne, G.Ciccotti, and D.F.Coker, Eds.
 World Scientific, Singapore, 1998
- 84-P) S.Cozzini, L.F.Rull, G.Ciccotti, and G.V.Paolini
"Intrinsic frame transport for a model of nematic liquid crystal"
 Physica A, 240, 173 (1997)
- 83-P) M.Ferrario, A.Fiorina, and G.Ciccotti
"Long time tails in two-dimensional fluids by MD"
 Physica A, 240, 268 (1997)
- 82) S.Melchionna, and G.Ciccotti
"Atomic stress isobaric scaling for systems subjected to holonomic constraints"
 J.Chem.Phys., 106, 195 (1997)
- 81) S.Melchionna, M.Barteri, and G.Ciccotti
"MD of microperoxidases in aqueous and non-aqueous solutions"
 J.Phys.Chem., 19241, 100 (1996)
- 80-B) G.Ciccotti, and M.Ferrario
"MD simulation of rare events: calculation of rate constants"
 In: **"MC and MD of condensed matter systems"**
 Euroconference 1995
 K.Binder and G.Ciccotti, Eds.
 SIF, 1996
- 79) S.Melchionna, G.Ciccotti, and B.L.Holian
"Comment on: Constant pressure molecular dynamics algorithms"
 J.Chem.Phys., 105, 346 (1996)
- 78) S.Bonella, G.Ciccotti, and D.Coker
"Research note on semiclassical limit in the intermediate scattering function"
 Mol.Phys., 89, 1203 (1996)
- 77) D.Laria, R.Kapral, D.Estrin, and G.Ciccotti

“MD study of solvation effects on acid dissociation in aprotic media”
J.Chem.Phys., 104, 1 (1996)

76-B) G.Ciccotti, M.Ferrario, D.Laria, and R.Kapral
“Simulation of classical and quantum activated processes in the condensed phase”
In: **“Progress in computational physics of matter: methods, software and applications”**
L.Reatto and F.Manghi, Eds.
World Scientific, Singapore, 1995

75) M.H.Mueser, and G.Ciccotti
“Two-dimensional orientational motion as a multichannel reaction by computer simulation”
J.Chem.Phys., 103, 4273 (1995)

74) D.Gravina, G.Ciccotti, and B.L.Holian,
“Linear and nonlinear viscous flow in two-dimensional fluids”
Phys.Rev.E, 52, 6123 (1995)

73) S.Melchionna, M.Barteri, and G.Ciccotti
“Molecular Dynamics study of monomeric haem undecapeptide of cytochrome C”
J. of Computer-aided Materials Design, 2, 9 (1995)

72) H.Luo, G.Ciccotti, M.Mareschal, M.Meyer, and B.Zappoli
“Thermal relaxation of supercritical fluids by equilibrium molecular dynamics”
Phys.Rev.E, 51, 2013 (1995)

1994 - 1990

71) M.Ferrario, D.Laria, G.Ciccotti, and R.Kapral
“Quantum effects on the solvent contribution to the activation free energy”
J. of Mol.Liq., 61, 37 (1994)

70-P) D.Laria, G.Ciccotti, M.Ferrario, and R.Kapral
“Proton transfer in solution”
In: **“Lectures on Thermodynamics and Statistical Mechanics”**
Proceedings of XXII Winter Meeting in Statistical Physics, Oaxtepec, Mexico
M.Lopez de Haro, and C.Varea, Eds.
World Scientific, Singapore, 1994

69) D.Laria, G.Ciccotti, M.Ferrario, and R.Kapral
“Activation free energy for proton transfer in solution”
Chem.Phys., 180, 181 (1994)

68) J.M.Depaepe, J.P.Ryckaert, E.Paci, and G.Ciccotti
“Sampling of molecular conformations by Molecular Dynamics technique”
Mol.Phys., 79, 515 (1993)

67) G.V.Paolini, G.Ciccotti, and M.Ferrario
“Simulation of site-site soft-core liquid crystal models”
Mol.Phys., 80, 297 (1993)

- 66) S.Melchionna, G.Ciccotti, and B.L.Holian
"Hoover's style Molecular Dynamics for systems varying in shape and size"
Mol.Phys., 78, 533 (1993)
- 65-B) G.Ciccotti, C.Pierleoni, and J.P.Ryckaert
"Theoretical foundations and rheological applications of nonequilibrium molecular dynamics"
In: **"Microscopic Simulations of Complex Hydrodynamic Phenomena"**
M.Mareschal, and B.L.Holian, Eds.
Plenum Press, New York, 1992
- 64) D.Laria, G.Ciccotti, M.Ferrario, and R.Kapral
"Molecular Dynamics study of adiabatic proton transfer reactions in solution"
J.Chem.Phys., 97, 378 (1992)
- 63) W.Loose, and G.Ciccotti
"Temperature and temperature control in nonequilibrium molecular dynamics simulations of the shear flow of dense liquids"
Phys.Rev.A, 45, 3859 (1992)
- 62) E.Paci, and G.Ciccotti
"Vacancy migration rates by molecular dynamics with constraints"
J. of Phys.: Condensed Matter, 4, 2173 (1992)
- 61) M.Ferrario, G.Ciccotti, B.L.Holian, and J.P.Ryckaert
"Shear-rate dependence of the viscosity of Argon at triple point"
Phys.Rev.A, 44, 6936 (1991)
- 60-B) G.Ciccotti
"Molecular Dynamics simulations of nonequilibrium phenomena and rare dynamical events"
In: **"Computer Simulation in Material Science: Interatomic potentials, Techniques and Applications"**
M.Meyer, and V.Pontikis, Eds.
Kluwer Academic Publishers, Dordrecht, 1991
- 59) E.Paci, G.Ciccotti, M.Ferrario, and R.Kapral
"Activation energies by molecular dynamics with constraints"
Chem.Phys.Lett. 176, 581 (1991)
- 58-B) M.Ferrario, G.Ciccotti, J.T.Hynes, and R.Kapral
"Molecular Dynamics Simulation on Supercomputers of Chemical Reactions in Solution"
In: **"Supercomputing Tools for Science and Engineering"**
D.Laforenza, and R.Perego, Eds.
Franco Angeli Libri, Milano, 1990
- 57) G.Ciccotti, M.Ferrario, J.T.Hynes, and R.Kapral
"Dynamics of Ion Pair Interconversion in a Polar Solvent"
J.Chem.Phys., 93, 7137 (1990)

- 56) G.V.Paolini, G.Ciccotti, and H.Van Beijeren
 “Nonequilibrium Molecular Dynamics via a Nondiverging Subtraction Technique”
 Phys.Rev.A, 42, 5912 (1990)
- 55-P) G.Ciccotti
 “The Nonexistence of Nonlinear Laws for Simple Fluids by Nonequilibrium Molecular Dynamics”
 In: “**Microscopic Simulations of Complex Flows**”
 M.Mareschal, Ed.
 Plenum Press, New York, 1990
- 54-B) G.Ciccotti
 “Computer Simulation of Equilibrium and Nonequilibrium Molecular Dynamics”
 In: “**Liquids, Freezing and Glass transition**”
 J.P.Hansen, D.Levesque, and J.Zinn-Justin, Eds.
 Elsevier Science Publishers, Amsterdam, 1990
- 53-P) J.T.Hynes, E.A.Carter, G.Ciccotti, M.Ferrario, and R.Kapral
 “Environmental Dynamics and Electron Transfer Reactions”
 In: “**Perspectives in Photosynthesis**”
 J.Jortner, and B.Pullman, Eds.
 Kluwer, 1990
- 52) C.Pierleoni, and G.Ciccotti
 “Thermotransport coefficients of a classical binary ionic mixture by nonequilibrium Molecular Dynamics”
 J. of Phys.: Condensed Matter, 2, 1315 (1990)
- 1989 - 1985**
- 51) D.A.Zichi, G.Ciccotti, J.T.Hynes, and M.Ferrario
 “Molecular Dynamics simulation of e-transfer reactions in solution”
 J. of Phys.Chem.: lett. sect., 93, 6261 (1989)
- 50) B.L.Holian, G.Ciccotti, W.G.Hoover, B.Moran, and H.A.Posch
 “Nonlinear-response theory for time-independent fields: consequences of the fractal nonequilibrium distribution function”
 Phys.Rev.A, 39, 5414 (1989)
- 49) E.A.Carter, G.Ciccotti, J.T.Hynes, and R.Kapral
 “Constrained reaction coordinate dynamics for the simulation of rare events”
 Chem.Phys.Lett., 156, 472 (1989)
- 48) R.Vogelsang, C.Hoheisel, P.Sindzingre, G.Ciccotti, and D.Frenkel
 “Computation of partial enthalpies of various Lennard-Jones mixtures by NPT Molecular Dynamics”
 J. of Phys.: Condensed Matter, 1, 957 (1989)
- 47) J.P.Ryckaert, A.Bellemans, G.Ciccotti, and G.V.Paolini

“The evaluation of transport coefficients of simple fluids by Molecular Dynamics: comparison of Green-Kubo and non-equilibrium approaches for shear viscosity”
Phys.Rev.A, 39, 259 (1989)

46) G.Ciccotti, M.Ferrario, J.T.Hynes, and R.Kapral
“Constrained Molecular Dynamics and the mean potential for an ion pair in a polar solvent”
Chem.Phys., 129, 241 (1989)

45) P.Sindzingre, C.Massobrio, G.Ciccotti, and D.Frenkel
“Calculation of partial enthalpies of an Argon-Krypton mixture by NPT Molecular Dynamics”
Chem.Phys., 129, 213 (1989)

44) C.Massobrio, V.Pontikis, and G.Ciccotti
“Diffusion in the LJ glass model by equilibrium and nonequilibrium MD”
Phys.Rev.B, 39, 2640 (1989)

43) C.Massobrio, V.Pontikis, and G.Ciccotti
“MD study of the atomic diffusion in glasses induced by an external perturbation”
Europhys.Lett., 5, 677 (1988)

42) M.Hayoun, M.Meyer, M.Mareschal, G.Ciccotti, and P.Turq
“Molecular Dynamics simulation of a liquid-liquid interface”
In: **“Chemical reactivity in Liquids: Fundamental aspects”**
M.Moreau, and P.Turq, Eds.
Plenum Press, New York, 1988

41) G.Ciccotti, M.Ferrario, J.T.Hynes, and R.Kapral
“Molecular Dynamics simulation of ion association reactions in a polar solvent”
J. de Chimie Phys. (Paris), 85, 925 (1988)

40) P.Turq, J.L.Fernandez-Abascal, and G.Ciccotti
“Brownian Dynamics of chemical reactions”
In: **“Chemical reactivity in Liquids: Fundamental aspects”**
M.Moreau, and P.Turq, Eds.
Plenum Press, New York, 1988

39) A.Bellemans, J.P.Ryckaert, G.Ciccotti, and G.V.Paolini
“The shear rate dependence of the viscosity of simple fluids by molecular dynamics”
Phys.Rev.Lett., 60, 128 (1988)

38) C.Pierleoni, G.Ciccotti, and B.Bernu
“Thermal conductivity of the classical one-component plasma by non-equilibrium molecular-dynamics”
Europhys.Lett., 4, 1115 (1987)

37) G.Ciccotti, M.Ferrario, E.Memeo, and M.Meyer
“Structural transition on cooling of plastic adamantane: a molecular-dynamics study”
Phys.Rev.Lett., 59, 2574 (1987)

- 36) G.Ciccotti, W.G.Hoover, C.Massobrio, and G.V.Paolini
“Dense-fluid transport coefficients via the constrained subtraction technique”
Phys.Rev.A, 36, 3471 (1987)
- 35) R.Vogelsang, C.Hoheisel, G.V.Paolini, and G.Ciccotti
“Soret coefficient of isotopic Lennard-Jones mixtures and the Ar-Kr system as determined by equilibrium molecular dynamics”
Phys.Rev.A, 36, 3964 (1987)
- 34) P.Sindzingre, G.Ciccotti, C.Massobrio, and D.Frenkel
“Partial enthalpies and related quantities in mixtures from computer simulations”
Chem.Phys.Lett., 136, 35 (1987)
- 33) R.Vogelsang, C.Hoheisel, and G.Ciccotti
“Thermal conductivity of the Lennard-Jones Liquid by molecular dynamics calculations”
J.Chem.Phys., 86, 6371 (1987)
- 32) G.V.Paolini, and G.Ciccotti
“Cross thermotransport in Liquid mixtures by nonequilibrium molecular dynamics”
Phys.Rev.A, 35, 5156 (1987)
- 31) G.Ciccotti, and J.P.Ryckaert
“Molecular Dynamics simulation of rigid molecules”
Comp.Phys.Rep., 3, 345 (1986) (Review)
- 30) G.V.Paolini, G.Ciccotti, and C.Massobrio
“Non-Linear thermal response of a LJ fluid near its triple point”
Phys.Rev.A, 34, 1355 (1986)
- 29) M.Meyer, C.Marhic, and G.Ciccotti
“Molecular Dynamics simulation of plastic adamantane. II. Reorientation motion”
Mol.Phys., 58, 723 (1986)
- 28) J.P.Ryckaert, and G.Ciccotti
“Andersen's canonical-ensemble molecular dynamics for molecules with constraints”
Mol.Phys., 58, 1125 (1986)
- 27) V.Rosato, G.Ciccotti, and V.Pontikis
“Molecular Dynamics study of surface premelting effects”
Phys.Rev.B, 33, 1860 (1986)
- 26) W.G.Hoover, G.Ciccotti, G.V.Paolini, and C.Massobrio
“Lennard-Jones triple-point conductivity via weak external fields: Additional calculations”
Phys.Rev.A, 32, 3765 (1985)
- 25-P) V.Rosato, V.Pontikis, and G.Ciccotti
“Cooperative Premelting Effects on a (110) fcc surface: a Molecular Dynamics study”
Proceed.Mat.Res.Soc.Symp., 63, 241 (1985)

24) M.Meyer, and G.Ciccotti
“*Molecular Dynamics simulation of plastic Adamantane. I. Structural Properties*”
Mol.Phys., 56, 1235 (1985)

1984 - 1980

23) C.Massobrio, and G.Ciccotti
“*Lennard-Jones triple-point conductivity via weak external fields*”
Phys.Rev.A, 30, 3191 (1984)

22) M.Guillopé, G.Ciccotti, and V.Pontikis
“*Relations between intergranular diffusion and structure: a molecular dynamics study*”
Surface Science, 144, 67 (1984)

21) G.Ciccotti, P.Turq, and F.Lantelme
“*Cluster approach to ion association reactions in electrolyte solutions*”
Chem.Phys., 88, 333 (1984)

20) C.Trozzi, and G.Ciccotti
“*Stationary non-equilibrium states by molecular dynamics. II. Newton's Law*”
Phys.Rev.A, 29, 916 (1984)

19) G.Ciccotti, and G.Ferrari
“*Was Poincare a herald of quantum theory?*”
European J. of Phys., 4, 110 (1983)

18) J.P.Ryckaert, and G.Ciccotti
“*Introduction of Andersen's demon in the molecular dynamics of systems with constraints*”
J.Chem.Phys., 78, 7368 (1983)

17) G.Ciccotti, M.Guillopé, and V.Pontikis
“*High-angle grain-boundary premelting transition: a molecular dynamics study*”
Phys.Rev.B, 22, 5576 (1983)

16) A.Tenenbaum, G.Ciccotti, and R.Gallico
“*Stationary non-equilibrium states by molecular dynamics. Fourier's Law*”
Phys.Rev.A, 25, 2778 (1982)

15) G.Ciccotti, M.Ferrario, and J.P.Ryckaert
“*Molecular dynamics of rigid systems in cartesian coordinates. A general formulation*”
Mol.Phys., 47, 1253 (1982)

14) G.Ciccotti, M.Ferrario, and J.P.Ryckaert
“*Computer simulation of the generalized brownian motion. II. An argon particle in Argon Fluid*”
Mol.Phys., 46, 875 (1982)

13) J.P.Ryckaert, A.Bellemans, and G.Ciccotti
“*The Rotation-Translation coupling in diatomic molecules*”

Mol.Phys., 44, 979 (1981)

12) G.Ciccotti, and J.P.Ryckaert

“On the derivation of the generalized Langevin equation for interacting brownian particles”
J.Stat.Phys., 26, 73 (1981)

11) G.Ciccotti, and A.Tenenbaum

“Canonical Ensemble and Nonequilibrium States by Molecular Dynamics”
J.Stat.Phys., 23, 767 (1980)

10) G.Ciccotti, and J.P.Ryckaert

“Computer simulation of the generalized brownian motion. I. The scalar case”
Mol.Phys., 40, 141 (1980)

1979 - 1975

9) G.Ciccotti, G.Jacucci, and I.R.McDonald

“Thought~Experiments by Molecular Dynamics”
J. of Stat.Phys., 21, 1 (1979)

8) G.Ciccotti, G.Jacucci, and I.R.McDonald

“Thermal Response to a weak external field”
J. of Phys.C, 11, 509 (1978)

7) J.P.Ryckaert, G.Ciccotti, and H.J.C.Berendsen

“Numerical integration of the Cartesian equation of motion of a system with constraints: molecular dynamics of N-alkanes”
J. of Computational Physics, 23, 327 (1977)

6) G.Ciccotti, G.Jacucci, and I.R.McDonald

“Transport properties of molten alkali halides”
Phys.Rev.A, 123, 426 (1976)

5) G.Ciccotti, and G.Jacucci

“Direct computation of dynamical response by molecular dynamics: the mobility of a charged Lennard-Jones particle”
Phys.Rev.Lett., 35, 789 (1975)

1974 - 1969

4) G.Ciccotti, and G.Jona-Lasinio

“The modern epistemological debate and the socialization of sciences”
Scientia, 108, 481 (1973)

3) D.Capocaccia, M.Cassandro, and G.Ciccotti

“Equilibrium states of an Ising ferromagnet in the low temperature region”
Commun.Math.Phys., 29, 31 (1973)

2) D.Capocaccia, G.Ciccotti, and C.Di Castro
“Some consequences of sum rules in the dynamic scaling approach”
Phys.Lett., 32A, 359 (1970)

1) D.Capocaccia, and G.Ciccotti
“Sum Rules for π -N scattering in the backward direction”
Nuovo Cimento, 61A, 369 (1969)

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BOOKS

- B8) “*Molecular Dynamics Simulation*”
Printed Edition of the Special *Entropy* Issue
G.Ciccotti, M.Ferrario, and C.Schuette, Eds.
MDPI, Basel, Beijing, 2014
- B7) “*Constraints: From physical principles to molecular simulations and beyond*”
Special Topics issue of the European Physical Journal,
P.Echenique, and G.Ciccotti, Eds.
Springer, Berlin, 2011
- B6) “*Computer Simulations in Condensed Matter: From Materials to Chemical Biology*”
M.Ferrario, G.Ciccotti, and K.Binder, Eds.
LNP Voll. 1&2, Springer, Berlin, 2006
- B5) “*Bridging time scales: Molecular simulations for the next decade*”
SIMU Conference, Konstanz 2001
P.Nielaba, M.Mareschal, and G.Ciccotti, Eds.
Springer, Berlin, 2003
- B4) “*Simulation of classical and quantum dynamics in condensed phase*”
Euroconference 1997
B.J.Berne, G.Ciccotti, and D.F.Coker, Eds.
World Scientific, Singapore, 1998
- B3) “*MC and MD of condensed matter systems*”
Euroconference 1995
K.Binder, and G.Ciccotti, Eds.
SIF, Bologna, 1996
- B2) “*Simulation of Liquids and Solids. Molecular Dynamics and MonteCarlo methods in Statistical Mechanics. A reprint book.*”

G.Ciccotti, D.Frenkel, and I.R.McDonald, Eds.
North Holland, Amsterdam, 1987

- B1) *“Molecular Dynamics Simulation of Statistical Mechanical Systems”*
“E.Fermi” SFI Summer School 1985
G.Ciccotti, and W.G.Hoover, Eds.
North Holland, Amsterdam, 1986

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LEGEND

P = Proceedings of a conference

B = Contribution to a book, either Summer School or Collective book

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