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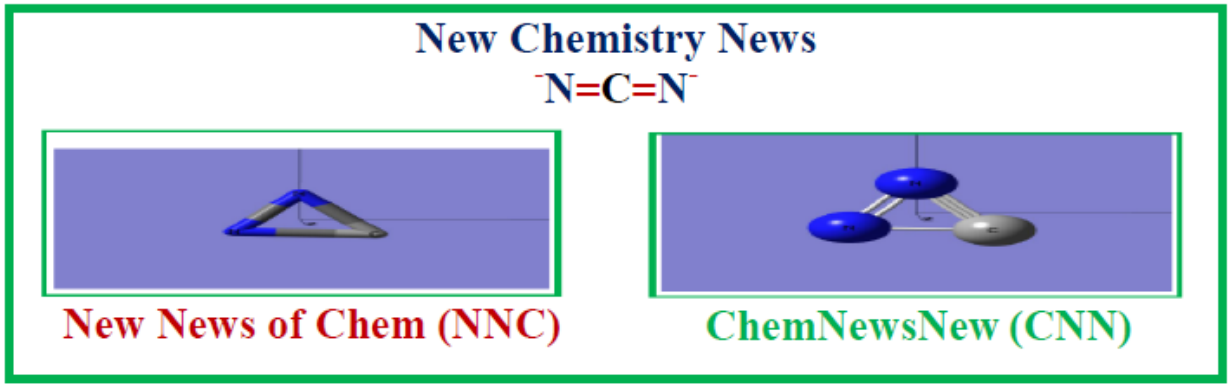

Meta Molecular Dynamics (MMD)

Transition-Tempered Metadynamics: Robust, Convergent Metadynamics via On-the-Fly Transition Barrier Estimation — J. Chem. Theory Comput., 2014, 10 (9), 3626–3633

James F. Dama, Grant Rotskoff**, Michele Parrinello**, and Gregory A. Voth

Flexible Docking in Solution Using Metadynamics — J. Am. Chem. Soc., 2005, 127 (8), 2600–2607

Francesco Luigi Gervasio, Alessandro Laio, and **Michele Parrinello**

Assessing the Accuracy of Metadynamics — J. Phys. Chem. B, 2005, 109 (14), 6714–6721

Alessandro Laio, Antonio Rodriguez-Fortea, Francesco Luigi Gervasio, Matteo Ceccarelli, and **Michele Parrinello**

Path Integral Metadynamics — J. Chem. Theory Comput., 2015, 11 (4), 1383–1388

Ruge Quhe, Marco Nava, Pratyush Tiwary, and Michele Parrinello

Assessing the Reliability of the Dynamics Reconstructed from Metadynamics — J. Chem. Theory Comput., 2014, 10 (4), 1420–1425

Matteo Salvalaglio, Pratyush Tiwary, and Michele Parrinello

Combustion Chemistry via Metadynamics: Benzyl Decomposition Revisited — J. Phys. Chem. A, 2015, 119 (6), 978–989

Daniela Polino and Michele Parrinello

Efficient Reconstruction of Complex Free Energy Landscapes by Multiple Walkers Metadynamics — J. Phys. Chem. B, 2006, 110 (8), 3533–3539

Paolo Raiteri, Alessandro Laio, Francesco Luigi Gervasio, Cristian Micheletti, and Michele Parrinello

Metadynamics with Adaptive Gaussians — J. Chem. Theory Comput., 2012, 8 (7), 2247–2254

Davide Branduardi, Giovanni Bussi, and Michele Parrinello

Dimer Metadynamics
J. Chem. Theory Comput., 2017, 13 (2), 425–430
Marco Nava , Ferruccio Palazzesi, Claudio Perego, and Michele Parrinello

A Time-Independent Free Energy Estimator for Metadynamics
J. Phys. Chem. B, 2015, 119 (3), 736–742
Pratyush Tiwary and Michele Parrinello

Flexible Docking in Solution Using Metadynamics
J. Am. Chem. Soc., 2005, 127 (8), 2600–2607
Francesco Luigi Gervasio, Alessandro Laio, and Michele Parrinello

Metadynamics with Adaptive Gaussians
Davide Branduardi, Giovanni Bussi, and Michele Parrinello

Efficient Sampling of High-Dimensional Free-Energy Landscapes with Parallel Bias Metadynamics
J. Chem. Theory Comput., 2015, 11 (11), 5062–5067
Jim Pfaendtner and Massimiliano Bonomi

Molecular Dynamics in the Multicanonical Ensemble: Equivalence of Wang–Landau Sampling, Statistical Temperature Molecular Dynamics, and Metadynamics
J. Chem. Theory Comput., 2014, 10 (5), 1843–1847
Christoph Junghans, Danny Perez, and Thomas Vogel

Transition-Tempered Metadynamics Is a Promising Tool for Studying the Permeation of Drug-like Molecules through Membranes
J. Chem. Theory Comput., 2016, 12 (10), 5157–5169
Rui Sun, James F. Dama, Jeffrey S. Tan, John P. Rose, and Gregory A. Voth

Merging Metadynamics into Hyperdynamics: Accelerated Molecular Simulations Reaching Time Scales from Microseconds to Seconds
J. Chem. Theory Comput., 2015, 11 (10), 4545–4554
Kristof M. Bal and Erik C. Neyts

Altruistic Metadynamics: Multisystem Biased Simulation
J. Phys. Chem. B, 2016, 120 (9), 2209–2215
Petr Hošek, Daniela Toulcová, Andrea Bortolato, and Vojtěch Spiwok

SAXS-Guided Metadynamics
J. Chem. Theory Comput., 2015, 11 (7), 3491–3498
Dari Kimanius, Ingrid Pettersson, Gerd Schluckebier, Erik Lindahl, and Magnus Andersson

Replica-Averaged Metadynamics
J. Chem. Theory Comput., 2013, 9 (12), 5610–5617
Carlo Camilloni, Andrea Cavalli, and Michele Vendruscolo

μ-tempered metadynamics: Artifact independent convergence times for wide hills
The Journal of Chemical Physics 143, 234109 (2015);
Bradley M. Dicksona)

Well-Tempered Metadynamics as a Tool for Characterizing Multi-Component, Crystalline Molecular Machines
J. Phys. Chem. B, 2013, 117 (40), 12286–12295
Andrew J. Ilott, Sebastian Palucha, Paul Hodgkinson, and Mark R. Wilson

Metadynamics in Essential Coordinates: Free Energy Simulation of Conformational Changes
J. Phys. Chem. B, 2007, 111 (12), 3073–3076
Vojtěch Spiwok, Petra Lipovová, and Blanka Králová

Metadynamics-Biased ab Initio Molecular Dynamics Study of Heterogeneous CO2 Reduction via Surface Frustrated Lewis Pairs — ACS Catal., 2016, 6 (10), 7109–7117

Mireille Ghoussoub, Shwetank Yadav, Kulbir Kaur Ghuman, Geoffrey A. Ozin, and Chandra Veer Singh

Deprotonation of Solvated Formic Acid: Car−Parrinello and Metadynamics Simulations — J. Phys. Chem. B, 2006, 110 (5), 2325–2331

Jung-Goo Lee, Eliana Asciutto, Volodymyr Babin, Celeste Sagui, Thomas Darden, and Christopher Roland

Assessing Generic Collective Variables for Determining Reaction Rates in MetadynamicsSimulations — J. Chem. Theory Comput., Article ASAP DOI: 10.1021/acs.jctc.7b00038

Christopher D. Fu, Luiz F. L. Oliveira, and Jim Pfaendtner

Empirical Corrections to the Amber RNA Force Field with Target Metadynamics — J. Chem. Theory Comput., 2016, 12 (6), 2790–2798

Alejandro Gil-Ley, Sandro Bottaro, and Giovanni Bussi

Conformational Free Energy Modeling of Druglike Molecules by Metadynamics in the WHIM Space — J. Chem. Inf. Model., 2012, 52 (3), 804–813

Vojtěch Spiwok, Katarína Hlat-Glembová, Igor Tvaroška, and Blanka Králová

Exploring Intramolecular Reactions in Complex Systems with Metadynamics: The Case of the Malonate Anions — J. Phys. Chem. A, 2005, 109 (34), 7682–7687

Eliana Asciutto and Celeste Sagui

ATP Hydrolysis Mechanism in a Maltose Transporter Explored by QM/MM Metadynamics Simulation — J. Phys. Chem. B, 2016, 120 (43), 11102–11112

Wei-Lin Hsu, Tadaomi Furuta, and Minoru Sakurai

Adenosine Triphosphate Hydrolysis Mechanism in Kinesin Studied by Combined Quantum-Mechanical/Molecular-Mechanical Metadynamics Simulations — J. Am. Chem. Soc., 2013, 135 (24), 8908–8919

J. Am. Chem. Soc., 2013, 135 (24), 8908–8919

Exploring the Folding Free Energy Landscape of Insulin Using Bias Exchange Metadynamics — J. Phys. Chem. B, 2009, 113 (11), 3556–3564

Nevena Todorova, Fabrizio Marinelli, Stefano Piana and Irene Yarovsky

Bias-Exchange Metadynamics Simulations: An Efficient Strategy for the Analysis of Conduction and Selectivity in Ion Channels — J. Chem. Theory Comput., 2015, 11 (4), 1896–1906

Carmen Domene, Paolo Barbini, and Simone Furini

The Role of Hydrogen Bonding in the Decomposition of H2CO3 in Water: Mechanistic Insights from Ab Initio Metadynamics Studies of Aqueous Clusters — J. Phys. Chem. B, 2014, 118 (22), 5983–5993

Mirza Galib and Gabriel Hanna

Statistical Mechanics of the Denatured State of a Protein Using Replica-Averaged Metadynamics — J. Am. Chem. Soc., 2014, 136 (25), 8982–8991

Carlo Camilloni and Michele Vendruscolo

Reaction Mechanisms of Water Splitting and H2 Evolution by a Ru(II)-Pincer Complex Identified with Ab Initio Metadynamics Simulations — ACS Catal., 2012, 2 (7), 1500–1506

Changru Ma, Simone Piccinin, and Stefano Fabris

Protonation of a Hydroxide Anion Bridging Two Divalent Magnesium Cations in Water Probed by First-Principles Metadynamics Simulation — J. Phys. Chem. B, 2010, 114 (34), 11102–11109

Jung Mee Park and Mauro Boero

Isomerism of Trimeric Aluminum Complexes in Aqueous Environments: Exploration via DFT-Based Metadynamics Simulation — J. Phys. Chem. B, 2016, 120 (45), 11800–11809

Giorgio Lanzani#, Ari P. Seitsonen, Marcella Iannuzzi, Kari Laasonen‖, and Simo O. Pehkonen⊥

Ab Initio Molecular Dynamics Simulations of Amino Acids in Aqueous Solutions: Estimating pKaValues from Metadynamics Sampling Anil Kumar Tummanapelli and Sukumaran Vasudevan	J. Phys. Chem. B, 2015, 119 (37), 12249–12255
Ab Initio MD Simulations of the Brønsted Acidity of Glutathione in Aqueous Solutions: Predicting pKa Shifts of the Cysteine Residue Anil Kumar Tummanapelli and Sukumaran Vasudevan	J Phys Chem B 119 (49), 15353-15358. 2015
Metadynamics As a Tool for Mapping the Conformational and Free-Energy Space of Peptides — The Alanine Dipeptide Case Study Jiří Vymětal and Jiří Vondrášek	J. Phys. Chem. B, 2010, 114 (16), 5632–5642
Metadynamics for Perspective Drug Design: Computationally Driven Synthesis of New Protein–Protein Interaction Inhibitors Targeting the EphA2 Receptor Matteo Incerti, Simonetta Russo, Donatella Callegari , Daniele Pala , Carmine Giorgio, Ilaria Zanotti, Elisabetta Barocelli, Paola Vicini, Federica Vacondio, Silvia Rivara , Riccardo Castelli, Massimiliano Tognolini , and Alessio Lodola	J. Med. Chem., 2017, 60 (2), 787–796
Mechanistic Insights into the Dissociation and Decomposition of Carbonic Acid in Water via the Hydroxide Route: An Ab Initio Metadynamics Study Mirza Galib and Gabriel Hanna	J. Phys. Chem. B, 2011, 115 (50), 15024–15035
Collective Proton Dynamics at Highly Charged Interfaces Studied by Ab Initio Metadynamics Swati Vartak, Ata Roudgar, Anatoly Golovnev, and Michael Eikerling	J. Phys. Chem. B, 2013, 117 (2), 583–588
Conformational Changes in the Epidermal Growth Factor Receptor: Role of the Transmembrane Domain Investigated by Coarse-Grained MetaDynamics Free Energy Calculations Mickaël Lelimousin, Vittorio Limongelli, and Mark S. P. Sansom	J. Am. Chem. Soc., 2016, 138 (33), 10611–10622
Exploring the Free Energy Landscape of Solutes Embedded in Lipid Bilayers Joakim P. M. Jämbeck and Alexander P. Lyubartsev	J. Phys. Chem. Lett., 2013, 4 (11), 1781–1787

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Object Oriented Vocabulary of Molecular Dynamics (MD) of chemical systems (CS)		
Systems	:	[Interacting, non-interacting]
Interacting systems	:	[Irreversible, reversible]
Reversible		[equilibrium, quasi-static]
Interacting systems as a function of time	:	[Chemical kinetics, Molecular Dynamics (MD), Meta MD]
Chemical kinetics	:	

		[Slow, Fast]
Molecular Dynamics	:	[Classical, ab initio]
Accelerated MD	:	[Hyperdynamics ; Parallel-replica dynamics ; Temperature accelerated dynamics]
Meta MD	:	[Altruistic; Bias parallel; Bias-exchange; Gaussians -adaptive; Hyperdynamics; Metropolis–hastings; Multiple walkers; Path integral; Replica-averaged; SAXS-guided; Tempered;]
Tempered meta MD		[Collective-variable tempering; μ-tempered; Well-tempered; Transition-tempered; Parallel tempered]

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