Massimo Mella

List of Publications by Year
in descending order

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82	1,442	331670 21	377865 34
papers	citations	h-index	g-index

84	84	84	1321
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	On the Chemistry of Ethanol on Basic Oxides: Revising Mechanisms and Intermediates in the Lebedev and Guerbet reactions. ChemSusChem, 2015, 8, 377-388.	6.8	158
2	Methanol as a clean and efficient H-transfer reactant for carbonyl reduction: Scope, limitations, and reaction mechanism. Journal of Catalysis, 2014, 317, 206-219.	6.2	70
3	Study of the Structure, Energetics, and Vibrational Properties of Small Ammonia Clusters (NH3)n (n =) Tj ETQq1 1 0.784314 rgBT /Ov	2.5	60
4	Modulating Antimicrobial Activity by Synthesis: Dendritic Copolymers Based on Nonquaternized 2-(Dimethylamino)ethyl Methacrylate by Cu-Mediated ATRP. Biomacromolecules, 2012, 13, 833-841.	5.4	58
5	Zero temperature quantum properties of small protonated water clusters (H2O)nH+ (n=1â€“5). Journal of Chemical Physics, 2003, 119, 10048-10062.	3.0	54
6	Quantum Monte Carlo investigation of small 4He clusters with a 3He impurity. Journal of Chemical Physics, 2000, 112, 717-722.	3.0	49
7	Mechanistic insights into the catalytic transfer hydrogenation of furfural with methanol and alkaline earth oxides. Journal of Catalysis, 2019, 372, 61-73.	6.2	44
8	Nuclear quantum effects on the structure and energetics of (H2O)6H+. Physical Chemistry Chemical Physics, 2005, 7, 2324.	2.8	40
9	Structure and Energetics of Ammonia Clusters (NH₃)_n (n = 3â^’20) Investigated Using a Rigidâ^’Polarizable Model Derived from ab Initio Calculations. Journal of Physical Chemistry A, 2008, 112, 2888-2898.	2.5	39
10	Predicting atomic dopant solvation in helium clusters: The MgHen case. Journal of Chemical Physics, 2005, 123, 054328.	3.0	38
11	Ground state and excitation dynamics in Ag doped helium clusters. Journal of Chemical Physics, 2002, 117, 9695-9702.	3.0	35
12	Communication: Nucleation of quantized vortex rings in 4He nanodroplets. Journal of Chemical Physics, 2014, 140, 131101.	3.0	29
13	Novel hydrogen- and halogen-bonding anion receptors based on 3-iodopyridinium units. RSC Advances, 2016, 6, 67540-67549.	3.6	29
14	Three-Fragment Counterpoise Correction of Potential Energy Curves for Proton-Transfer Reactions. Journal of Physical Chemistry A, 2003, 107, 7589-7596.	2.5	28
15	Influence of charged intramolecular hydrogen bonds in weak polyelectrolytes: A Monte Carlo study of flexible and extendible polymeric chains in solution and near charged spheres. Journal of Polymer Science, Part B: Polymer Physics, 2015, 53, 650-663.	2.1	28
16	Role of the Metal Center in the Ethylene Polymerization Promoted by Group 4 Complexes Supported by a Tetradentate [OSSO]-Type Bis(phenolato) Ligand. ACS Catalysis, 2011, 1, 1460-1468.	11.2	26
17	The Role of Charge Density and Hydrophobicity on the Biocidal Properties of Selfâ€Protonable Polymeric Materials. Macromolecular Bioscience, 2015, 15, 927-940.	4.1	26
18	Escherichia coli as a Model for the Description of the Antimicrobial Mechanism of a Cationic Polymer Surface: Cellular Target and Bacterial Contrast Response. ACS Applied Materials & Interfaces, 2019, 11, 15332-15343.	8.0	26

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19	Modulation of ionization and structural properties of weak polyelectrolytes due to 1D, 2D, and 3D confinement. Journal of Polymer Science, Part B: Polymer Physics, 2017, 55, 1088-1102.	2.1	26
20	Quantum Monte Carlo simulations of selected ammonia clusters (nÂ=Â2â€“5): Isotope effects on the ground state of typical hydrogen bonded systems. Journal of Chemical Physics, 2010, 133, 214301.	3.0	24
21	A cascade mechanism for a simple reaction: The gas-phase methylation of phenol with methanol. Journal of Catalysis, 2019, 370, 447-460.	6.2	23
22	Mg/Ga mixed-oxide catalysts for phenol methylation: Outstanding performance in 2,4,6-trimethylphenol synthesis with co-feeding of water. Applied Catalysis A: General, 2018, 552, 86-97.	4.3	22
23	Impact of Charge Correlation, Chain Rigidity, and Chemical Specific Interactions on the Behavior of Weak Polyelectrolytes in Solution. Journal of Physical Chemistry B, 2019, 123, 8872-8888.	2.6	21
24	Thermodynamic properties of ammonia clusters (NH3)nâ€ˆn=2â€“11: Comparing classical and quantum simulation results for hydrogen bonded species. Journal of Chemical Physics, 2009, 131, 034312.	3.0	20
25	Solubility of Metal Atoms in Helium Droplets: Exploring the Effect of the Well Depth Using the Coinage Metals Cu and Ag. Journal of Physical Chemistry A, 2011, 115, 7141-7152.	2.5	20
26	Comparison of different propagators in diffusion Monte Carlo simulations of noble gas clusters. Journal of Chemical Physics, 2003, 119, 5601-5606.	3.0	19
27	Absorbed weak polyelectrolytes: Impact of confinement, topology, and chemically specific interactions on ionization, conformation free energy, counterion condensation, and absorption equilibrium. Journal of Polymer Science, Part B: Polymer Physics, 2019, 57, 491-510.	2.1	19
28	Structural properties of hydrophilic polymeric chains bearing covalentlyâ€“linked hydrophobic substituents: Exploring the effects of chain length, fractional loading and hydrophobic interaction strength with coarse grained potentials and Monte Carlo simulations. Polymer, 2010, 51, 3582-3589.	3.8	18
29	Monte Carlo study of the effects of macroion charge distribution on the ionization and adsorption of weak polyelectrolytes and concurrent counterion release. Journal of Colloid and Interface Science, 2020, 560, 667-680.	9.4	18
30	Alternative Low-Energy Mechanisms for Isotopic Exchange in Gas-Phase D2O-H+(H2O)nReactions. ChemPhysChem, 2006, 7, 894-903.	2.1	17
31	Improved diffusion Monte Carlo propagators for bosonic systems using ItÃ´ calculus. Journal of Chemical Physics, 2006, 125, 184106.	3.0	16
32	Improved diffusion Monte Carlo for bosonic systems using time-step extrapolation â€œon the flyâ€• Journal of Chemical Physics, 2007, 126, 104106.	3.0	15
33	Dynamics of photoexcited Ba+ cations in 4He nanodroplets. Journal of Chemical Physics, 2016, 144, 094302.	3.0	15
34	Importance sampling for quantum Monte Carlo in manifolds: Addressing the time scale problem in simulations of molecular aggregates. Journal of Chemical Physics, 2008, 128, 164102.	3.0	14
35	Higher order diffusion Monte Carlo propagators for linear rotors as diffusion on a sphere: Development and application to O2@Hen. Journal of Chemical Physics, 2011, 135, 114504.	3.0	14
36	â€œLeaching or not leachingâ€• an alternative approach to antimicrobial materials via copolymers containing crown ethers as active groups. Biomaterials Science, 2017, 5, 741-751.	5.4	14

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37	Hydrogen Transfer Activation via Stabilization of Coordinatively Vacant Sites: Tuning Long-Range Ï€-System Electronic Interaction between Ru(0) and NHC Pendants. Organometallics, 2019, 38, 1041-1051.	2.3	14
38	Quantum simulations of the hydrogen molecule on ammonia clusters. Journal of Chemical Physics, 2013, 139, 124319.	3.0	13
39	Quantum monte carlo methods for constrained systems. International Journal of Quantum Chemistry, 2014, 114, 611-625.	2.0	12
40	Out of Equilibrium Self-Assembly of Janus Nanoparticles: Steering It from Disordered Amorphous to 2D Patterned Aggregates. Langmuir, 2016, 32, 12934-12946.	3.5	11
41	Reactivity of a Cationic Alkyl Amino-Functionalized Cyclopentadienyl Aluminum Compound with Olefins: NMR Observation and Computational Investigation of the Single Propene Insertion Product into an Alâ‹¯C Bond. Organometallics, 2009, 28, 2554-2562.	2.3	10
42	Exciplexes with Ionic Dopants: Stability, Structure, and Experimental Relevance of M+(2P)4Hen (M = Sr,) Tj ETQq0 0 0 rgBT /Overlock 10	2.3	10
43	On the convergence of diffusion Monte Carlo in non-Euclidean spaces. I. Free diffusion. Journal of Chemical Physics, 2015, 142, 114110.	3.0	10
44	Impact of intermolecular drug-copolymer interactions on size and drug release kinetics from pH-responsive polymersomes. Supramolecular Chemistry, 2017, 29, 796-807.	1.2	10
45	The competition between dehydrogenation and dehydration reactions for primary and secondary alcohols over gallia: unravelling the effects of molecular and electronic structure via a two-pronged theoretical/experimental approach. Catalysis Science and Technology, 2020, 10, 3433-3449.	4.1	10
46	Coinage metal exciplexes with helium atoms: a theoretical study of M*(2L)Hen (M = Cu, Ag, Au; L = P,D). Physical Chemistry Chemical Physics, 2013, 15, 18410.	2.8	9
47	On the convergence of diffusion Monte Carlo in non-Euclidean spaces. II. Diffusion with sources and sinks. Journal of Chemical Physics, 2015, 142, 114111.	3.0	9
48	Exploring unvisited regions to investigate solution properties: The backyard of H3O+ and its aggregates. Chemical Physics Letters, 2013, 555, 51-56.	2.6	8
49	Inducing pH control over the critical micelle concentration of zwitterionic surfactants via polyacids adsorption: Effect of chain length and structure. Journal of Colloid and Interface Science, 2022, 606, 1636-1651.	9.4	8
50	On possible simplifications in the theoretical description of gas phase atomic cluster dissociation. Journal of Chemical Physics, 2009, 130, 084108.	3.0	7
51	Assessment of the Effects of Anisotropic Interactions among Hydrogen Molecules and Their Isotopologues: A Diffusion Monte Carlo Investigation of Gas Phase and Adsorbed Clusters. Journal of Physical Chemistry A, 2017, 121, 5005-5017.	2.5	7
52	On the origin and consequences of high DMAEMA reactivity ratio in ATRP copolymerization with MMA: An experimental and theoretical study[#]. Journal of Polymer Science Part A, 2018, 56, 1366-1382.	2.3	7
53	Synthesis, crystal structure, and optical properties of fluorinated poly(pyrazole) ligands andin silicoassessment of their affinity for volatile organic compounds. New Journal of Chemistry, 2020, 44, 6443-6455.	2.8	7
54	Effect of the cluster angular momentum J and the projectile orbital momentum L on capture probability and postcollision dynamics. Journal of Chemical Physics, 2009, 131, 124309.	3.0	6

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55	Dicopper(II) Mozobil^{TM}: a dinuclear receptor for the pyrophosphate anion in aqueous solution. Supramolecular Chemistry, 2017, 29, 834-845.	1.2	6
56	Synthesis and Spectroscopic Characterization of 2-(het)Aryl Perimidine Derivatives with Enhanced Fluorescence Quantum Yields. Journal of Fluorescence, 2019, 29, 495-504.	2.5	6
57	On the distribution of hydrophilic polyelectrolytes and their counterions around zwitterionic micelles: the possible impact on the charge density in solution. Soft Matter, 2021, 17, 1267-1283.	2.7	6
58	Can oppositely charged polyelectrolyte stars form a gel? A simulational study. Soft Matter, 2021, 17, 1574-1588.	2.7	6
59	Evidences for charged hydrogen bonds on surfaces bearing weakly basic pendants: The case of PMMAâ€“ranâ€“PDMAEMA polymeric films. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2021, 620, 126525.	4.7	6
60	Efficient calculation of low energy statistical rates for gas phase dissociation using umbrella sampling. Journal of Chemical Physics, 2006, 124, 104302.	3.0	5
61	Pathways for hydrogen bond switching in a tetrameric methanol cluster. Physical Chemistry Chemical Physics, 2009, 11, 11340.	2.8	5
62	An analytical potential energy model for ammoniaâ€“H2 from first principle. Chemical Physics Letters, 2012, 535, 49-55.	2.6	5
63	Interpreting â€œAcidityâ€•as a Global Property Controlling Comonomer Reactivity in Olefin Polymerization. Organometallics, 2013, 32, 3192-3202.	2.3	5
64	Replica exchange Hybrid Monte Carlo simulations of the ammonia dodecamer and hexadecamer. Chemical Physics Letters, 2015, 635, 127-133.	2.6	5
65	Quest for Inexpensive Hydrogen Isotopic Fractionation: Do We Need 2D Quantum Confining in Porous Materials or Are Rough Surfaces Enough? The Case of Ammonia Nanoclusters. Journal of Physical Chemistry A, 2016, 120, 8148-8159.	2.5	5
66	Diffusion Monte Carlo simulations of gas phase and adsorbed D2-(H2)n clusters. Journal of Chemical Physics, 2018, 148, 102315.	3.0	5
67	Interface Counterion Localization Induces a Switch between Tight and Loose Configurations of Knotted Weak Polyacid Rings despite Intermonomer Coulomb Repulsions. Journal of Physical Chemistry B, 2020, 124, 2930-2937.	2.6	5
68	Tunable Knot Segregation in Copolyelectrolyte Rings Carrying a Neutral Segment. ACS Macro Letters, 2021, 10, 1365-1370.	4.8	5
69	Discretization error-free estimate of low temperature statistical dissociation rates in gas phase: Applications to Lennard-Jones clusters X13â^nYn (n=0â€“3). Journal of Chemical Physics, 2008, 128, 244515.	3.0	4
70	Infinite swapping in curved spaces. Journal of Chemical Physics, 2014, 140, 014103.	3.0	4
71	Improved importance sampling distribution for rate constant calculation. Journal of Chemical Physics, 2005, 122, 204106.	3.0	3
72	Macroscopic evidences for non-Rice-Ramsperger-Kassel effects in the reaction between H3O+ and D2O: The occurrence of nonstatistical isotopic branching ratio. Journal of Chemical Physics, 2007, 126, 204305.	3.0	3

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73	Replica exchange with Smart Monte Carlo and Hybrid Monte Carlo in manifolds. Chemical Physics Letters, 2013, 590, 214-220.	2.6	3
74	Impact of Chemically Specific Interactions between Anions and Weak Polyacids on Chain Ionization, Conformations, and Solution Energetics. Macromolecules, 2022, 55, 4533-4547.	4.8	3
75	Controlling Drug Release of Anti-inflammatory Molecules Through a pH-Sensitive, Bactericidal Polymer Matrix: Towards a Synergic and Combined Therapy. Lecture Notes in Bioengineering, 2020, , 151-163.	0.4	2
76	Interaction between surfaces decorated with like-charged pendants: Unravelling the interplay between energy and entropy leading to attraction. Journal of Colloid and Interface Science, 2022, 619, 51-64.	9.4	2
77	Quantum Monte Carlo: Direct Determination of the Difference between True and Trial Wavefunctions. Recent Advances in Computational, 1997, , 21-38.	0.8	1
78	How Chemical Structure and Composition Impact on the Release of Salt-like Drugs from Hydrophobic Matrices: Variation of Mechanism upon Adding Hydrophilic Features to PMMA. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, , 128878.	4.7	1
79	Asymmetric Phenyl Substitution: An Effective Strategy to Enhance the Photosensitizing Potential of Curcuminoids. Pharmaceuticals, 2022, 15, 843.	3.8	1
80	Electronic Quantum Monte Carlo Calculations of Energies and Atomic Forces for Diatomic and Polyatomic Molecules. ACS Symposium Series, 2006, , 69-79.	0.5	0
81	Quantum Monte Carlo Approaches for Tackling Electronic Correlation. , 2011, , 237-269.		0
82	Composition and Microstructure of Biocompatible and pH-Sensitive Copolymers Prepared by a Free Solvent ARGET ATRP. Lecture Notes in Bioengineering, 2020, , 3-15.	0.4	0