Emiliano Ippoliti

List of Publications by Year
in descending order

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37 papers	914 citations	471509 17 h-index	477307 29 g-index
38 all docs	38 docs citations	38 times ranked	1385 citing authors

#	Article	IF	Citations
1	Wavefunction-Based Electrostatic-Embedding QM/MM Using CFOUR through MiMiC. Journal of Chemical Theory and Computation, 2022, 18, 13-24.	5.3	2
2	Mechanisms Underlying Proton Release in CLC-type F^{â€“}/H⁺ Antiporters. Journal of Physical Chemistry Letters, 2021, 12, 4415-4420.	4.6	10
3	Machine Learning of Allosteric Effects: The Analysis of Ligand-Induced Dynamics to Predict Functional Effects in TRAP1. Journal of Physical Chemistry B, 2021, 125, 101-114.	2.6	20
4	All-Atom Simulations Disclose How Cytochrome Reductase Reshapes the Substrate Access/Egress Routes of Its Partner CYP450s. Journal of Physical Chemistry Letters, 2020, 11, 1189-1193.	4.6	18
5	MiMiC: Multiscale Modeling in Computational Chemistry. Frontiers in Molecular Biosciences, 2020, 7, 45.	3.5	5
6	Molecular Basis of CLC Antiporter Inhibition by Fluoride. Journal of the American Chemical Society, 2020, 142, 7254-7258.	13.7	20
7	Extreme Scalability of DFT-Based QM/MM MD Simulations Using MiMiC. Journal of Chemical Theory and Computation, 2019, 15, 5601-5613.	5.3	32
8	MiMiC: A Novel Framework for Multiscale Modeling in Computational Chemistry. Journal of Chemical Theory and Computation, 2019, 15, 3810-3823.	5.3	31
9	Post-Translational Regulation of CYP450s Metabolism As Revealed by All-Atoms Simulations of the Aromatase Enzyme. Journal of Chemical Information and Modeling, 2019, 59, 2930-2940.	5.4	22
10	Proton Dynamics in Protein Mass Spectrometry. Journal of Physical Chemistry Letters, 2017, 8, 1105-1112.	4.6	34
11	Designing the Sniper: Improving Targeted Human Cytolytic Fusion Proteins for Anti-Cancer Therapy via Molecular Simulation. Biomedicines, 2017, 5, 9.	3.2	8
12	A Self-Activated Mechanism for Nucleic Acid Polymerization Catalyzed by DNA/RNA Polymerases. Journal of the American Chemical Society, 2016, 138, 14592-14598.	13.7	56
13	Chapter 9. First Principles Methods in Biology: From Continuum Models to Hybrid Ab initio Quantum Mechanics/Molecular Mechanics. RSC Theoretical and Computational Chemistry Series, 2016, , 294-339.	0.7	4
14	Structure and Dynamics of Oligonucleotides in the Gas Phase. Angewandte Chemie - International Edition, 2015, 54, 467-471.	13.8	26
15	Molecular Simulation-Based Structural Prediction of Protein Complexes in Mass Spectrometry: The Human Insulin Dimer. PLoS Computational Biology, 2014, 10, e1003838.	3.2	13
16	Hydration of chloride anions in the NanC Porin fromEscherichia coli:A comparative study by QM/MM and MD simulations. Journal of Chemical Physics, 2014, 141, 22D521.	3.0	3
17	Structural Biology of Cisplatin Complexes with Cellular Targets: The Adduct with Human Copper Chaperone Atox1 in Aqueous Solution. Chemistry - A European Journal, 2014, 20, 11719-11725.	3.3	14
18	Platination of the copper transporter ATP7A involved in anticancer drug resistance. Dalton Transactions, 2014, 43, 12085.	3.3	29

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19	Molecular Recognition of Platinated DNA from Chromosomal HMGB1. Journal of Chemical Theory and Computation, 2014, 10, 3578-3584.	5.3	12
20	Ion Permeation in the NanC Porin from Escherichia coli: Free Energy Calculations along Pathways Identified by Coarse-Grain Simulations. Journal of Physical Chemistry B, 2013, 117, 13534-13542.	2.6	6
21	Role of the Membrane Dipole Potential for Proton Transport in Gramicidin A Embedded in a DMPC Bilayer. Journal of Chemical Theory and Computation, 2013, 9, 3826-3831.	5.3	17
22	Structural prediction of a rhodamine-based biosensor and comparison with biophysical data. Physical Chemistry Chemical Physics, 2013, 15, 2177-2183.	2.8	12
23	Theoretical optical spectroscopy of complex systems. Journal of Electron Spectroscopy and Related Phenomena, 2013, 189, 46-55.	1.7	7
24	Conformational Fluctuations of UreG, an Intrinsically Disordered Enzyme. Biochemistry, 2013, 52, 2949-2954.	2.5	33
25	Structural Determinants of Cisplatin and Transplatin Binding to the Met-Rich Motif of Ctr1: A Computational Spectroscopy Approach. Journal of Chemical Theory and Computation, 2012, 8, 2912-2920.	5.3	27
26	Counterion Redistribution upon Binding of a Tat-Protein Mimic to HIV-1 TAR RNA. Journal of Chemical Theory and Computation, 2012, 8, 688-694.	5.3	24
27	Water at hydrophobic interfaces delays proton surface-to-bulk transfer and provides a pathway for lateral proton diffusion. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 9744-9749.	7.1	104
28	Manyâ€body meets QM/MM: Application to indole in water solution. Physica Status Solidi (B): Basic Research, 2010, 247, 1920-1924.	1.5	3
29	Bioinorganic Chemistry of Parkinsonâ€™s Disease: Structural Determinants for the Copper-Mediated Amyloid Formation of Alpha-Synuclein. Inorganic Chemistry, 2010, 49, 10668-10679.	4.0	119
30	Spectroscopic Properties of Formaldehyde in Aqueous Solution: Insights from Carâ€'Parrinello and TDDFT/CASPT2 Calculations. Journal of Chemical Theory and Computation, 2010, 6, 3403-3409.	5.3	7
31	Many-Body Perturbation Theory Extended to the Quantum Mechanics/Molecular Mechanics Approach: Application to Indole in Water Solution. Journal of Chemical Theory and Computation, 2009, 5, 1822-1828.	5.3	13
32	Geometric phase for open quantum systems and stochastic unravelings. Physical Review A, 2006, 73, .	2.5	35
33	Dynamical reduction models and the energy conservation principle. AIP Conference Proceedings, 2006, , .	0.4	1
34	Towards quantum superpositions of a mirror: an exact open systems analysisâ€"calculational details. Journal of Physics A, 2005, 38, 2715-2727.	1.6	29
35	On the energy increase in space-collapse models. Journal of Physics A, 2005, 38, 8017-8038.	1.6	46
36	Towards Quantum Superpositions of a Mirror: An Exact Open Systems Analysis. Physical Review Letters, 2005, 94, 030401.	7.8	56

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37	Numerical analysis of a spontaneous collapse model for a two-level system. Physical Review A, 2004, 69, .	2.5	16