Sebastian Thallmair

List of Publications by Year
in descending order

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42 papers	1,599 citations	394421 19 h-index	330143 37 g-index
48 all docs	48 docs citations	48 times ranked	1400 citing authors

#	Article	IF	Citations
1	Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388.	19.0	557
2	Pitfalls of the Martini Model. Journal of Chemical Theory and Computation, 2019, 15, 5448-5460.	5.3	159
3	Proteinâ€“ligand binding with the coarse-grained Martini model. Nature Communications, 2020, 11, 3714.	12.8	139
4	Optimal control theory â€“ closing the gap between theory and experiment. Physical Chemistry Chemical Physics, 2012, 14, 14460.	2.8	63
5	Molecular dynamics simulations in photosynthesis. Photosynthesis Research, 2020, 144, 273-295.	2.9	50
6	Complete and incomplete spin transitions in 1D chain iron(<scp>ii</scp>) compounds. New Journal of Chemistry, 2011, 35, 691-700.	2.8	49
7	An Allosteric Pathway in Copper, Zinc Superoxide Dismutase Unravels the Molecular Mechanism of the G93A Amyotrophic Lateral Sclerosis-Linked Mutation. Journal of Physical Chemistry Letters, 2019, 10, 7740-7744.	4.6	49
8	Unidirectional rotating molecular motors dynamically interact with adsorbed proteins to direct the fate of mesenchymal stem cells. Science Advances, 2020, 6, eaay2756.	10.3	42
9	Cholesterol Flip-Flop Impacts Domain Registration in Plasma Membrane Models. Journal of Physical Chemistry Letters, 2018, 9, 5527-5533.	4.6	36
10	Controlling Photorelaxation in Uracil with Shaped Laser Pulses: AÂTheoretical Assessment. Journal of the American Chemical Society, 2017, 139, 5061-5066.	13.7	35
11	Capturing Cholineâ€“Aromatics Cationâ^Ï€ Interactions in the MARTINI Force Field. Journal of Chemical Theory and Computation, 2020, 16, 2550-2560.	5.3	35
12	Lipid Fingerprints and Cofactor Dynamics of Light-Harvesting Complex II in Different Membranes. Biophysical Journal, 2019, 116, 1446-1455.	0.5	31
13	Nonconverged Constraints Cause Artificial Temperature Gradients in Lipid Bilayer Simulations. Journal of Physical Chemistry B, 2021, 125, 9537-9546.	2.6	28
14	Computational Redesign of an Ï‰-Transaminase from Pseudomonas jessenii for Asymmetric Synthesis of Enantiopure Bulky Amines. ACS Catalysis, 2021, 11, 10733-10747.	11.2	28
15	Chemoselective quantum control of carbonyl bonds in Grignard reactions using shaped laser pulses. Physical Chemistry Chemical Physics, 2010, 12, 15780.	2.8	22
16	Ionâ€Pairing of Phosphonium Salts in Solution: Cï£¿Hâ‹…â‹…â‹…Halogen and Cï£¿Hâ‹…â‹…â‹…Ï€ Hydrogen Bonds. Chemistry - A European Journal, 2013, 19, 14612-14630.	3.3	22
17	A Comprehensive Microscopic Picture of the Benzhydryl Radical and Cation Photogeneration and Interconversion through Electron Transfer. ChemPhysChem, 2013, 14, 1423-1437.	2.1	22
18	Design of specially adapted reactive coordinates to economically compute potential and kinetic energy operators including geometry relaxation. Journal of Chemical Physics, 2016, 144, 234104.	3.0	21

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19	Martini 3 Coarse-Grained Model for Type III Deep Eutectic Solvents: Thermodynamic, Structural, and Extraction Properties. ACS Sustainable Chemistry and Engineering, 2021, 9, 17338-17350.	6.7	20
20	Quantum Dynamics in an Explicit Solvent Environment: A Photochemical Bond Cleavage Treated with a Combined QD/MD Approach. Journal of Chemical Theory and Computation, 2015, 11, 1987-1995.	5.3	19
21	Quantum Dynamics of a Photochemical Bond Cleavage Influenced by the Solvent Environment: A Dynamic Continuum Approach. Journal of Physical Chemistry Letters, 2014, 5, 3480-3485.	4.6	18
22	Computational Prediction of Ï‰-Transaminase Specificity by a Combination of Docking and Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2021, 61, 5569-5580.	5.4	17
23	Two New Methods To Generate Internal Coordinates for Molecular Wave Packet Dynamics in Reduced Dimensions. Journal of Chemical Theory and Computation, 2016, 12, 5698-5708.	5.3	14
24	A multi target approach to control chemical reactions in their inhomogeneous solvent environment. Journal of Physics B: Atomic, Molecular and Optical Physics, 2015, 48, 234003.	1.5	13
25	Simulating the control of molecular reactions via modulated light fields: from gas phase to solution. Journal of Physics B: Atomic, Molecular and Optical Physics, 2017, 50, 082001.	1.5	12
26	Perspective: a stirring role for metabolism in cells. Molecular Systems Biology, 2022, 18, e10822.	7.2	12
27	Strategies towards the purposeful design of long-range ferromagnetic ordering due to spin canting. Polyhedron, 2009, 28, 1796-1801.	2.2	11
28	Hypothesis-Driven, Structure-Based Design in Photopharmacology: The Case of eDHFR Inhibitors. Journal of Medicinal Chemistry, 2022, 65, 4798-4817.	6.4	10
29	Ultrafast photochemistry with two product channels: Wavepacket motion through two distinct conical intersections. Chemical Physics Letters, 2017, 683, 128-134.	2.6	9
30	Biaryl sulfonamides as cisoid azosteres for photopharmacology. Chemical Communications, 2021, 57, 4126-4129.	4.1	9
31	Protein dynamics and lipid affinity of monomeric, zeaxanthin-binding LHCII in thylakoid membranes. Biophysical Journal, 2022, 121, 396-409.	0.5	9
32	Molecular features in complex environment: Cooperative team players during excited state bond cleavage. Structural Dynamics, 2016, 3, 043205.	2.3	7
33	Ultrafast Reactive Quantum Dynamics Coupled to Classical Solvent Dynamics Using an Ehrenfest Approach. Journal of Physical Chemistry A, 2018, 122, 2849-2857.	2.5	7
34	Ground and Excited State Surfaces for the Photochemical Bond Cleavage in Phenylmethylphenylphosphonium Ions. Journal of Physical Chemistry A, 2013, 117, 10626-10633.	2.5	6
35	Running in the Family: Molecular Factors controlling Spin Crossover of Iron(II) Complexes with Schiffâ€base like Ligands. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2021, 647, 905-914.	1.2	6
36	Small ionic radii limit time step in Martini 3 molecular dynamics simulations. Journal of Chemical Physics, 2022, 157, .	3.0	6

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37	The Interplay of Nuclear and Electron Wavepacket Motion in the Control of Molecular Processes: A Theoretical Perspective. Physical Chemistry in Action, 2014, , 213-248.	0.6	3
38	Molecular Dynamcis of Light-Harvesting Complex II Embedded in the Thylakoid Membrane. Biophysical Journal, 2018, 114, 522a.	0.5	0
39	Chromophore arrangement in light-harvesting complex II influenced by the protein dynamics on the microsecond time scale. EPJ Web of Conferences, 2019, 205, 09039.	0.3	0
40	Quantum Dynamics of Molecular Reactions Directed by Explicit Solvent Environment. , 2014, , .		0
41	Optimal Control Theory for Molecular Reactions in Atomistic Surroundings. , 2016, , .		0
42	How to Control the Ultrafast Dynamics of Uracil with Shaped Laser Pulses: Theoretical Insights. , 2016, , .		0