

Irmgard Frank

List of Publications by Year in descending order

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48
papers

996
citations

567281

15
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434195

31
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51
all docs

51
docs citations

51
times ranked

968
citing authors

#	ARTICLE	IF	CITATIONS
1	Classical nuclear motion: Does it fail to explain reactions and spectra in certain cases?. International Journal of Quantum Chemistry, 2022, 122, .	2.0	2
2	The First Reaction Steps of Lithium-Mediated Ammonia Synthesis: Ab Initio Simulation. Nitrogen, 2022, 3, 404-413.	1.3	1
3	Deterministic quantum mechanics: The role of the Maxwell-Boltzmann distribution. International Journal of Quantum Chemistry, 2021, 121, e26555.	2.0	6
4	Anionic Thia-Fries Rearrangement at Ferrocene: A Computational and Experimental Study. Helvetica Chimica Acta, 2021, 104, e2100025.	1.6	3
5	Ab-Initio Molecular Dynamics Simulation of the Electrolysis of Nucleobases. Energies, 2021, 14, 5021.	3.1	1
6	Ab-Initio Molecular Dynamics Simulation of Condensed-Phase Reactivity: The Electrolysis of Ammonia and Ethanamine in Aquatic Carbon Dioxide Solutions. Energies, 2021, 14, 6510.	3.1	0
7	Ammonia, water, and hydrogen: Can nuclear motion be described classically?. International Journal of Quantum Chemistry, 2020, 120, e26142.	2.0	4
8	Ab-Initio Molecular Dynamics Simulation of Condensed-Phase Reactivity: The Electrolysis of Amino Acids and Peptides. Molecules, 2020, 25, 5415.	3.8	3
9	Some simple facts about water: CPMD simulation. Molecular Physics, 2020, 118, e1802074.	1.7	0
10	First-Principles Simulation of Highly Reactive Systems: Immediacy on a Femtosecond Time Scale. ChemistrySelect, 2020, 5, 5109-5116.	1.5	0
11	Classical Motion of the Nuclei in a Molecule: A Concept Without Alternatives. ChemistrySelect, 2020, 5, 1872-1877.	1.5	0
12	Xe-OCS: relatively straightforward?. Physical Chemistry Chemical Physics, 2020, 22, 5615-5624.	2.8	4
13	Modelling Vibrational Dissociation of $[H_2^+HCO]^+$. ChemistrySelect, 2019, 4, 9794-9801.	1.5	1
14	Carbon Monoxide Playing Ping Pong with a Proton: The Movie. ChemistrySelect, 2019, 4, 868-872.	1.5	3
15	Ab-Initio Molecular Dynamics Simulation of the Electrolysis of Waste Water. ChemistrySelect, 2019, 4, 4376-4381.	1.5	4
16	Validating additive correction schemes against gradient-based extrapolations. International Journal of Quantum Chemistry, 2019, 119, e25953.	2.0	6
17	Constrained Chemical Dynamics of CO Dissociation/Hydrogenation on Rh Surfaces. Chemistry - A European Journal, 2018, 24, 7188-7199.	3.3	3
18	The tardy dance of molecular orbitals. International Journal of Quantum Chemistry, 2018, 118, e25718.	2.0	3

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19	Ladderenes: The mechanochemistry and the photochemistry of an exciting class of substances. <i>Chemical Physics Letters</i> , 2018, 702, 76-81.	2.6	3
20	A single-molecule reaction cascade: First-principles molecular dynamics simulation. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25395.	2.0	1
21	On the dynamics of H ₂ adsorption on the Pt(111) surface. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25407.	2.0	11
22	CPMD Simulation of a Bimolecular Chemical Reaction: Nucleophilic Attack of a Disulfide Bond under Mechanical Stress. <i>Chemistry - A European Journal</i> , 2012, 18, 16332-16338.	3.3	19
23	Electrolysis of Water in the Diffusion Layer: First-Principles Molecular Dynamics Simulation. <i>Chemistry - A European Journal</i> , 2012, 18, 277-282.	3.3	13
24	The Formation of DNA Photodamage: The Role of Exciton Localization. <i>ChemPhysChem</i> , 2010, 11, 2011-2015.	2.1	21
25	Conservation of Orbital Symmetry can be Circumvented in Mechanically Induced Reactions. <i>ChemPhysChem</i> , 2010, 11, 3339-3342.	2.1	15
26	Disulfide Bond Cleavage: A Redox Reaction Without Electron Transfer. <i>Chemistry - A European Journal</i> , 2010, 16, 5097-5101.	3.3	29
27	Carâ€Parrinello Molecular Dynamics Study of the Thermal Decomposition of Sodium Fulminate. <i>Chemistry - A European Journal</i> , 2010, 16, 8041-8046.	3.3	1
28	Restricted open-shell Kohnâ€Sham theory: N unpaired electrons. <i>Chemical Physics</i> , 2010, 373, 283-288.	1.9	5
29	Mechanism of Electrocyclic Ringâ€Opening of Diphenyloxirane: 40 Years after Woodward and Hoffmann. <i>Chemistry - A European Journal</i> , 2009, 15, 10825-10829.	3.3	15
30	Origins of Material Failure in Siloxane Elastomers from First Principles. <i>ChemPhysChem</i> , 2009, 10, 119-123.	2.1	15
31	Breaking bonds at a stretch. <i>Nature Chemistry</i> , 2009, 1, 180-181.	13.6	5
32	Breaking the rules. <i>Nature Chemistry</i> , 2009, 1, 264-265.	13.6	12
33	Excited state dynamics in pyrroleâ€water clusters: First-principles simulation. <i>Chemical Physics</i> , 2008, 343, 347-352.	1.9	16
34	Solving restricted open-shell equations in excited state molecular dynamics simulations. <i>Chemical Physics</i> , 2008, 347, 17-24.	1.9	14
35	Formation and decay of tetrazane derivativesâ€a Carâ€Parrinello molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 4383.	2.8	4
36	Restricted open-shell Kohn-Sham theory: Simulation of the pyrrole photodissociation. <i>Journal of Chemical Physics</i> , 2007, 126, 125105.	3.0	31

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37	Molecular origins of adhesive failure: Siloxane elastomers pulled from a silica surface. <i>Physical Review B</i> , 2007, 76, .	3.2	13
38	Modified Chemistry of Siloxanes under Tensile Stress:Â Interaction with Environment. <i>Journal of Physical Chemistry B</i> , 2006, 110, 14557-14563.	2.6	22
39	First-Principles Simulation of the Photoreaction of a Capped Azobenzene: The Rotational Pathway is Feasible. <i>ChemPhysChem</i> , 2006, 7, 1455-1461.	2.1	36
40	Light-Driven Unidirectional Rotation in a Molecule: ROKS Simulation. <i>ChemPhysChem</i> , 2005, 6, 1943-1947.	2.1	26
41	A Molecular Spring for Vision. <i>Journal of the American Chemical Society</i> , 2004, 126, 15328-15329.	13.7	98
42	Ultrafast Cold Reactions in the Bipropellant Monomethylhydrazine/Nitrogen Tetroxide: CPMD Simulations. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 4586-4589.	13.8	33
43	Chemische Reaktionen âœœon the flyâœ¸. <i>Angewandte Chemie</i> , 2003, 115, 1607-1609.	2.0	6
44	Restricted open-shell Kohnâ€Šam theory for $\tilde{\Gamma}$ â€Š $\tilde{\Gamma}^*$ transitions. I. Polyenes, cyanines, and protonated imines. <i>Journal of Chemical Physics</i> , 2003, 119, 11574-11584.	3.0	62
45	Restricted open-shell Kohnâ€Šam theory for $\tilde{\Gamma}$ â€Š $\tilde{\Gamma}^*$ transitions. II. Simulation of photochemical reactions. <i>Journal of Chemical Physics</i> , 2003, 119, 11585-11590.	3.0	34
46	Breaking Bonds by Mechanical Stress:âœ¸ When Do Electrons Decide for the Other Side?. <i>Journal of the American Chemical Society</i> , 2002, 124, 3402-3406.	13.7	80
47	First-principles molecular dynamics study of a polymer under tensile stress. <i>Journal of Chemical Physics</i> , 2001, 115, 8670-8674.	3.0	48
48	Molecular dynamics in low-spin excited states. <i>Journal of Chemical Physics</i> , 1998, 108, 4060-4069.	3.0	249