# Irmgard Frank

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/2332906/publications.pdf

Version: 2024-02-01

| 48 | 996 | 567281 | 434195 |
|---|---|---|---|
| papers | citations | 15 h-index | 31 g-index |

| 51 | 51 | 51 | 968 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Molecular dynamics in low-spin excited states. Journal of Chemical Physics, 1998, 108, 4060-4069. | 3.0 | 249 |
| 2 | A Molecular Spring for Vision. Journal of the American Chemical Society, 2004, 126, 15328-15329. | 13.7 | 98 |
| 3 | Breaking Bonds by Mechanical Stress:â€‰ When Do Electrons Decide for the Other Side?. Journal of the American Chemical Society, 2002, 124, 3402-3406. | 13.7 | 80 |
| 4 | Restricted open-shell Kohnâ€“Sham theory for Ï€âˆ—Ï€* transitions. I. Polyenes, cyanines, and protonated imines. Journal of Chemical Physics, 2003, 119, 11574-11584. | 3.0 | 62 |
| 5 | First-principles molecular dynamics study of a polymer under tensile stress. Journal of Chemical Physics, 2001, 115, 8670-8674. | 3.0 | 48 |
| 6 | First-Principles Simulation of the Photoreaction of a Capped Azobenzene: The Rotational Pathway is Feasible. ChemPhysChem, 2006, 7, 1455-1461. | 2.1 | 36 |
| 7 | Restricted open-shell Kohnâ€“Sham theory for Ï€âˆ—Ï€* transitions. II. Simulation of photochemical reactions. Journal of Chemical Physics, 2003, 119, 11585-11590. | 3.0 | 34 |
| 8 | Ultrafast Cold Reactions in the Bipropellant Monomethylhydrazine/Nitrogen Tetroxide: CPMD Simulations. Angewandte Chemie - International Edition, 2004, 43, 4586-4589. | 13.8 | 33 |
| 9 | Restricted open-shell Kohn-Sham theory: Simulation of the pyrrole photodissociation. Journal of Chemical Physics, 2007, 126, 125105. | 3.0 | 31 |
| 10 | Disulfide Bond Cleavage: A Redox Reaction Without Electron Transfer. Chemistry - A European Journal, 2010, 16, 5097-5101. | 3.3 | 29 |
| 11 | Light-Driven Unidirectional Rotation in a Molecule: ROKS Simulation. ChemPhysChem, 2005, 6, 1943-1947. | 2.1 | 26 |
| 12 | Modified Chemistry of Siloxanes under Tensile Stress:Â Interaction with Environment. Journal of Physical Chemistry B, 2006, 110, 14557-14563. | 2.6 | 22 |
| 13 | The Formation of DNA Photodamage: The Role of Exciton Localization. ChemPhysChem, 2010, 11, 2011-2015. | 2.1 | 21 |
| 14 | CPMD Simulation of a Bimolecular Chemical Reaction: Nucleophilic Attack of a Disulfide Bond under Mechanical Stress. Chemistry - A European Journal, 2012, 18, 16332-16338. | 3.3 | 19 |
| 15 | Excited state dynamics in pyrroleâ€“water clusters: First-principles simulation. Chemical Physics, 2008, 343, 347-352. | 1.9 | 16 |
| 16 | Mechanism of Electrocyclic Ringâ€Opening of Diphenyloxirane: 40 Years after Woodward and Hoffmann. Chemistry - A European Journal, 2009, 15, 10825-10829. | 3.3 | 15 |
| 17 | Origins of Material Failure in Siloxane Elastomers from First Principles. ChemPhysChem, 2009, 10, 119-123. | 2.1 | 15 |
| 18 | Conservation of Orbital Symmetry can be Circumvented in Mechanically Induced Reactions. ChemPhysChem, 2010, 11, 3339-3342. | 2.1 | 15 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Solving restricted open-shell equations in excited state molecular dynamics simulations. Chemical Physics, 2008, 347, 17-24. | 1.9 | 14 |
| 20 | Molecular origins of adhesive failure: Siloxane elastomers pulled from a silica surface. Physical Review B, 2007, 76, . | 3.2 | 13 |
| 21 | Electrolysis of Water in the Diffusion Layer: Firstâ€Principles Molecular Dynamics Simulation. Chemistry - A European Journal, 2012, 18, 277-282. | 3.3 | 13 |
| 22 | Breaking the rules. Nature Chemistry, 2009, 1, 264-265. | 13.6 | 12 |
| 23 | On the dynamics of H<sub>2</sub> adsorption on the Pt(111) surface. International Journal of Quantum Chemistry, 2017, 117, e25407. | 2.0 | 11 |
| 24 | Chemische Reaktionen â€œon the flyâ€• Angewandte Chemie, 2003, 115, 1607-1609. | 2.0 | 6 |
| 25 | Validating additive correction schemes against gradientâ€based extrapolations. International Journal of Quantum Chemistry, 2019, 119, e25953. | 2.0 | 6 |
| 26 | Deterministic quantum mechanics: The role of the Maxwellâ€“Boltzmann distribution. International Journal of Quantum Chemistry, 2021, 121, e26555. | 2.0 | 6 |
| 27 | Breaking bonds at a stretch. Nature Chemistry, 2009, 1, 180-181. | 13.6 | 5 |
| 28 | Restricted open-shell Kohnâ€“Sham theory: N unpaired electrons. Chemical Physics, 2010, 373, 283-288. | 1.9 | 5 |
| 29 | Formation and decay of tetrazane derivativesâ€”a Carâ€“Parrinello molecular dynamics study. Physical Chemistry Chemical Physics, 2008, 10, 4383. | 2.8 | 4 |
| 30 | Abâ€initio Molecular Dynamics Simulation of the Electrolysis of Waste Water. ChemistrySelect, 2019, 4, 4376-4381. | 1.5 | 4 |
| 31 | Ammonia, water, and hydrogen: Can nuclear motion be described classically?. International Journal of Quantum Chemistry, 2020, 120, e26142. | 2.0 | 4 |
| 32 | Xeâ‹¯OCS: relatively straightforward?. Physical Chemistry Chemical Physics, 2020, 22, 5615-5624. | 2.8 | 4 |
| 33 | Constrained Chemical Dynamics of CO Dissociation/Hydrogenation on Rh Surfaces. Chemistry - A European Journal, 2018, 24, 7188-7199. | 3.3 | 3 |
| 34 | The tardy dance of molecular orbitals. International Journal of Quantum Chemistry, 2018, 118, e25718. | 2.0 | 3 |
| 35 | Ladderenes: The mechanochemistry and the photochemistry of an exciting class of substances. Chemical Physics Letters, 2018, 702, 76-81. | 2.6 | 3 |
| 36 | Carbon Monoxide Playing Ping Pong with a Proton: The Movie. ChemistrySelect, 2019, 4, 868-872. | 1.5 | 3 |

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|---|---|---|---|
| 37 | Ab-Initio Molecular Dynamics Simulation of Condensed-Phase Reactivity: The Electrolysis of Amino Acids and Peptides. Molecules, 2020, 25, 5415. | 3.8 | 3 |
| 38 | Anionic Thiaâ€•Fries Rearrangement at Ferrocene: A Computational and Experimental Study. Helvetica Chimica Acta, 2021, 104, e2100025. | 1.6 | 3 |
| 39 | Classical nuclear motion: Does it fail to explain reactions and spectra in certain cases?. International Journal of Quantum Chemistry, 2022, 122, . | 2.0 | 2 |
| 40 | Carâ€“Parrinello Molecular Dynamics Study of the Thermal Decomposition of Sodium Fulminate. Chemistry - A European Journal, 2010, 16, 8041-8046. | 3.3 | 1 |
| 41 | A singleâ€molecule reaction cascade: Firstâ€principles molecular dynamics simulation. International Journal of Quantum Chemistry, 2017, 117, e25395. | 2.0 | 1 |
| 42 | Modelling Vibrational Dissociation of [H<sub>2</sub>â€“HCO]<sup>+</sup>. ChemistrySelect, 2019, 4, 9794-9801. | 1.5 | 1 |
| 43 | Ab-Initio Molecular Dynamics Simulation of the Electrolysis of Nucleobases. Energies, 2021, 14, 5021. | 3.1 | 1 |
| 44 | The First Reaction Steps of Lithium-Mediated Ammonia Synthesis: Ab Initio Simulation. Nitrogen, 2022, 3, 404-413. | 1.3 | 1 |
| 45 | Some simple facts about water: CPMD simulation. Molecular Physics, 2020, 118, e1802074. | 1.7 | 0 |
| 46 | Firstâ€Principles Simulation of Highly Reactive Systems: Immediacy on a Femtosecond Time Scale. ChemistrySelect, 2020, 5, 5109-5116. | 1.5 | 0 |
| 47 | Classical Motion of the Nuclei in a Molecule: A Concept Without Alternatives. ChemistrySelect, 2020, 5, 1872-1877. | 1.5 | 0 |
| 48 | Ab-Initio Molecular Dynamics Simulation of Condensed-Phase Reactivity: The Electrolysis of Ammonia and Ethanimine in Aquatic Carbon Dioxide Solutions. Energies, 2021, 14, 6510. | 3.1 | 0 |