Jacek Jakowski

List of Publications by Year
in descending order

65 papers	1,722 citations	279487 23 h-index	288905 40 g-index
66 all docs	66 docs citations	66 times ranked	2649 citing authors

#	Article	IF	Citations
1	Quantum theory of electronic excitation and sputtering by transmission electron microscopy. Nanoscale, 2023, 15, 1053-1067.	2.8	5
2	From classical to quantum dynamics of atomic and ionic species interacting with graphene and its analogue. Theoretical and Computational Chemistry, 2022, , 61-86.	0.2	0
3	From ground to excited electronic state dynamics of electron and ion irradiated graphene nanomaterials. Theoretical and Computational Chemistry, 2022, , 87-107.	0.2	0
4	Nonadiabatic Effects on Defect Diffusion in Silicon-Doped Nanographenes. Nano Letters, 2021, 21, 236-242.	4.5	10
5	Deuteration and Polymers: Rich History with Great Potential. Macromolecules, 2021, 54, 3555-3584.	2.2	31
6	Benchmarking Quantum Chemistry Computations with Variational, Imaginary Time Evolution, and Krylov Space Solver Algorithms. Advanced Quantum Technologies, 2021, 4, 2100012.	1.8	21
7	Harnessing autocatalytic reactions in polymerization and depolymerization. MRS Communications, 2021, 11, 377-390.	0.8	4
8	Electron-Beam-Induced Molecular Plasmon Excitation and Energy Transfer in Silver Molecular Nanowires. Journal of Physical Chemistry A, 2021, 125, 74-87.	1.1	3
9	Understanding Beam-Induced Electronic Excitations in Materials. Journal of Chemical Theory and Computation, 2020, 16, 1200-1214.	2.3	13
10	Damage-Free Nanoscale Isotopic Analysis of Biological Materials with Vibrational Electron Spectroscopy. Microscopy and Microanalysis, 2019, 25, 1088-1089.	0.2	0
11	A TD-DFT Treatment of Electronic Excitations in the STEM Spanning Dipole and Impact Scattering Regimes. Microscopy and Microanalysis, 2019, 25, 2300-2301.	0.2	0
12	Identification of site-specific isotopic labels by vibrational spectroscopy in the electron microscope. Science, 2019, 363, 525-528.	6.0	124
13	Electronically Nonadiabatic Structural Transformations Promoted by Electron Beams. Advanced Functional Materials, 2019, 29, 1901901.	7.8	12
14	Quantum chemistry as a benchmark for near-term quantum computers. Npj Quantum Information, 2019, 5, .	2.8	138
15	A fast scheme to calculate electronic couplings between P3HT polymer units using diabatic orbitals for charge transfer dynamics simulations. Journal of Computational Chemistry, 2019, 40, 532-542.	1.5	2
16	Multi-purposed Ar gas cluster ion beam processing for graphene engineering. Carbon, 2018, 131, 142-148.	5.4	18
17	Non-Transition-Metal Catalytic System for N₂ Reduction to NH₃: AÂDensity Functional Theory Study of Al-Doped Graphene. Journal of Physical Chemistry Letters, 2018, 9, 570-576.	2.1	43
18	Selectively Deuterated Poly(Îµ-caprolactone)s: Synthesis and Isotope Effects on the Crystal Structures and Properties. Macromolecules, 2018, 51, 9393-9404.	2.2	20

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19	Theoretical assessment of the nuclear quantum effects on polymer crystallinity via perturbation theory and dynamics. International Journal of Quantum Chemistry, 2018, 118, e25712.	1.0	3
20	Assessing the Predictive Power of Density Functional Theory in Finite-Temperature Hydrogen Adsorption/Desorption Thermodynamics. Journal of Physical Chemistry C, 2018, 122, 26189-26195.	1.5	5
21	An experimental and computational study of donorâ€“linkerâ€“acceptor block copolymers for organic photovoltaics. Journal of Polymer Science, Part B: Polymer Physics, 2018, 56, 1135-1143.	2.4	4
22	Nuclear quantum effects on adsorption of H2 and isotopologues on metal ions. Chemical Physics Letters, 2017, 670, 64-70.	1.2	12
23	Enhancing Ion Migration in Grain Boundaries of Hybrid Organicâ€“Inorganic Perovskites by Chlorine. Advanced Functional Materials, 2017, 27, 1700749.	7.8	74
24	Relevance of the Nuclear Quantum Effects on the Proton/Deuteron Transmission through Hexagonal Boron Nitride and Graphene Monolayers. Journal of Physical Chemistry C, 2017, 121, 24335-24344.	1.5	23
25	Deuteration as a Means to Tune Crystallinity of Conducting Polymers. Journal of Physical Chemistry Letters, 2017, 8, 4333-4340.	2.1	16
26	Building with ions: towards direct write of platinum nanostructures using in situ liquid cell helium ion microscopy. Nanoscale, 2017, 9, 12949-12956.	2.8	8
27	Perovskites: Enhancing Ion Migration in Grain Boundaries of Hybrid Organicâ€“Inorganic Perovskites by Chlorine (Adv. Funct. Mater. 26/2017). Advanced Functional Materials, 2017, 27, .	7.8	1
28	Effects of partial La filling and Sb vacancy defects on <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>CoS</mml:mi><mml:msub><mml:mi mathvariant="normal">b</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> skutterudites. Physical Review B, 2017, 95, .	1.1	26
29	Understanding How Isotopes Affect Charge Transfer in P3HT/PCBM: A Quantum Trajectory-Electronic Structure Study with Nonlinear Quantum Corrections. Journal of Chemical Theory and Computation, 2016, 12, 4487-4500.	2.3	11
30	A computational workflow for designing silicon donor qubits. Nanotechnology, 2016, 27, 424002.	1.3	3
31	Approximate quantum trajectory dynamics for reactive processes in condensed phase. Molecular Simulation, 2015, 41, 86-106.	0.9	7
32	Highly Energetic Collisions of Xe with Fullerene Clusters. , 2014, , .		0
33	The isotopic effects of deuteration on optoelectronic properties of conducting polymers. Nature Communications, 2014, 5, 3180.	5.8	103
34	The effect of local substrate motion on quantum hydrogen transfer in soybean lipoxygenase-1 modeled with QTES-DFTB dynamics. Chemical Physics Letters, 2014, 613, 104-109.	1.2	6
35	Adsorption of a Hydrogen Atom on a Graphene Flake Examined with Quantum Trajectory/Electronic Structure Dynamics. Journal of Physical Chemistry C, 2014, 118, 16175-16187.	1.5	14
36	The hybrid Quantum Trajectory/Electronic Structure DFTB-based approach to Molecular Dynamics. , 2014, , .		0

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37	The divideâ€“expandâ€“consolidate MP2 scheme goes massively parallel. Molecular Physics, 2013, 111, 1196-1210.	0.8	38
38	Quantum Trajectory-Electronic Structure Approach for Exploring Nuclear Effects in the Dynamics of Nanomaterials. Journal of Chemical Theory and Computation, 2013, 9, 5221-5235.	2.3	29
39	Deuterium Uptake in Magnetic-Fusion Devices with Lithium-Conditioned Carbon Walls. Physical Review Letters, 2013, 110, 105001.	2.9	45
40	Optimization of density functional tight-binding and classical reactive molecular dynamics for high-throughput simulations of carbon materials. , 2012, , .		1
41	MP2 energy and density for large molecular systems with internal error control using the Divide-Expand-Consolidate scheme. Physical Chemistry Chemical Physics, 2012, 14, 15706.	1.3	57
42	Description of proton transfer in soybean lipoxygenase-1 employing approximate quantum trajectory dynamics. Chemical Physics Letters, 2012, 542, 153-158.	1.2	12
43	Dynamics of deuterium retention and sputtering of Liâ€“Câ€“O surfaces. Fusion Engineering and Design, 2012, 87, 1732-1736.	1.0	20
44	Detection of hydrogen using graphene. Nanoscale Research Letters, 2012, 7, 198.	3.1	27
45	Advancing Understanding and Design of Functional Materials Through Theoretical and Computational Chemical Physics. , 2012, , 209-278.		3
46	Modeling Charge Transfer in Fullerene Collisions via Real-Time Electron Dynamics. Journal of Physical Chemistry Letters, 2012, 3, 1536-1542.	2.1	23
47	Time-dependent quantum dynamical simulations of C₂condensation under extreme conditions. Physical Chemistry Chemical Physics, 2012, 14, 6273-6279.	1.3	14
48	Quantum Chemistry. , 2011, , 59-73.		5
49	Collision-induced fusion of twoC60fullerenes: Quantum chemical molecular dynamics simulations. Physical Review B, 2010, 82, .	1.1	30
50	Implementation and benchmark tests of the DFTB method and its application in the ONIOM method. International Journal of Quantum Chemistry, 2009, 109, 1841-1854.	1.0	58
51	Liouvilleâ€“von Neumann molecular dynamics. Journal of Chemical Physics, 2009, 130, 224106.	1.2	43
52	13C CP MAS NMR and GIAO-CHF/DFT calculations of flavonoids: Morin, kaempferol, tricin, genistein, formononetin and 3,7-dihydroxyflavone. Journal of Molecular Structure, 2008, 873, 109-116.	1.8	26
53	Hydrogen Tunneling in an Enzyme Active Site: A Quantum Wavepacket Dynamical Perspective. Journal of Physical Chemistry B, 2008, 112, 7601-7613.	1.2	66
54	Possible mechanisms for protecting NCÎ± bonds in helical peptides from electron-capture (or transfer) dissociation. International Journal of Mass Spectrometry, 2007, 265, 197-212.	0.7	41

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55	Computational Improvements to Quantum Wave Packet ab Initio Molecular Dynamics Using a Potential-Adapted, Time-Dependent Deterministic Sampling Technique. Journal of Chemical Theory and Computation, 2006, 2, 1203-1219.	2.3	32
56	Catalytic Hydrodeoxygenation of Methyl-Substituted Phenols:Â Correlations of Kinetic Parameters with Molecular Properties. Journal of Physical Chemistry B, 2006, 110, 14283-14291.	1.2	203
57	Quantum wave packet ab initio molecular dynamics: An approach to study quantum dynamics in large systems. Journal of Chemical Physics, 2005, 122, 114105.	1.2	53
58	Conformational analysis of N-benzyl-N-o-tolyl-p-methylbenzene-sulfonamides from dynamic 1H NMR experiments and theoretical calculations. Computational and Theoretical Chemistry, 2004, 680, 5-13.	1.5	3
59	Theoretical Analysis of the Electronic Structure and Bonding Stability of the TCNE Dimer Dianion (TCNE)22-. Journal of the American Chemical Society, 2003, 125, 16089-16096.	6.6	68
60	Characterization of Ar[sub n]O[sup â˜] clusters from ab initio and diffusion Monte Carlo calculations. Journal of Chemical Physics, 2003, 118, 2748.	1.2	8
61	Modeling of the three-body effects in the Ar[sub 2]O[sup â˜] trimer from ab initio calculations. Journal of Chemical Physics, 2003, 118, 2731.	1.2	6
62	Modeling of the Three-Body Effects in the Neutral Trimers in the Quartet State by ab initio Calculations. H3, Na3, and Na2B. Collection of Czechoslovak Chemical Communications, 2003, 68, 587-626.	1.0	3
63	Ab initio based study of the ArOâ˜ photoelectron spectra: Selectivity of spinâ€“orbit transitions. Journal of Chemical Physics, 2000, 112, 5852-5865.	1.2	31
64	Structure and energetics of ArnNOâ˜ clusters from ab initio calculations. Journal of Chemical Physics, 2000, 112, 10895-10904.	1.2	7
65	Many-body exchange effects in clusters of rare gases with a chromophore: He2CO2. Chemical Physics, 1998, 239, 573-591.	0.9	6