Marlies Hankel

List of Publications by Year
in descending order

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63 papers	3,341 citations	159585 30 h-index	144013 57 g-index
64 all docs	64 docs citations	64 times ranked	4030 citing authors

#	Article	IF	Citations
1	Coordination of Atomic Coâ€“Pt Coupling Species at Carbon Defects as Active Sites for Oxygen Reduction Reaction. Journal of the American Chemical Society, 2018, 140, 10757-10763.	13.7	464
2	Graphdiyne: a versatile nanomaterial for electronics and hydrogen purification. Chemical Communications, 2011, 47, 11843.	4.1	329
3	Understanding the Origin of Li₂MnO₃ Activation in Liâ€Rich Cathode Materials for Lithiumâ€Ion Batteries. Advanced Functional Materials, 2015, 25, 7488-7496.	14.9	151
4	Evaluating the Catalytic Efficiency of Paired, Single-Atom Catalysts for the Oxygen Reduction Reaction. ACS Catalysis, 2019, 9, 7660-7667.	11.2	128
5	Enhanced CO2 photocatalytic reduction on alkali-decorated graphitic carbon nitride. Applied Catalysis B: Environmental, 2017, 216, 146-155.	20.2	127
6	Biphenylene and Phagraphene as Lithium Ion Battery Anode Materials. ACS Applied Materials & Interfaces, 2017, 9, 20577-20584.	8.0	122
7	Lithium and Sodium Storage on Graphitic Carbon Nitride. Journal of Physical Chemistry C, 2015, 119, 21921-21927.	3.1	115
8	Modelling carbon membranes for gas and isotope separation. Physical Chemistry Chemical Physics, 2013, 15, 4832.	2.8	95
9	Lithium storage on carbon nitride, graphenylene and inorganic graphenylene. Physical Chemistry Chemical Physics, 2016, 18, 14205-14215.	2.8	93
10	State-to-state reactive differential cross sections for the H+H2â†'H2+H reaction on five different potential energy surfaces employing a new quantum wavepacket computer code: DIFFREALWAVE. Journal of Chemical Physics, 2006, 125, 164303.	3.0	85
11	Capacitance-enhanced sodium-ion storage in nitrogen-rich hard carbon. Journal of Materials Chemistry A, 2017, 5, 22186-22192.	10.3	85
12	Asymmetrically Decorated, Doped Porous Graphene As an Effective Membrane for Hydrogen Isotope Separation. Journal of Physical Chemistry C, 2012, 116, 6672-6676.	3.1	81
13	Carbon Nitride Nanofibres with Exceptional Lithium Storage Capacity: From Theoretical Prediction to Experimental Implementation. Advanced Functional Materials, 2018, 28, 1803972.	14.9	77
14	Computational Evaluation of Lithium-Functionalized Carbon Nitride (g-C₆N₈) Monolayer as an Efficient Hydrogen Storage Material. Journal of Physical Chemistry C, 2016, 120, 25180-25188.	3.1	76
15	Design of a 1D/2D C3N4/rGO composite as an anode material for stable and effective potassium storage. Energy Storage Materials, 2020, 25, 495-501.	18.0	68
16	Sodium-intercalated bulk graphdiyne as an anode material for rechargeable batteries. Journal of Power Sources, 2017, 343, 354-363.	7.8	66
17	Graphenylene Monolayers Doped with Alkali or Alkaline Earth Metals: Promising Materials for Clean Energy Storage. Journal of Physical Chemistry C, 2017, 121, 14393-14400.	3.1	65
18	Theoretical and experimental investigations of mesoporous C3N5/MoS2 hybrid for lithium and sodium ion batteries. Nano Energy, 2020, 72, 104702.	16.0	65

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19	Hydrogenated defective graphene as an anode material for sodium and calcium ion batteries: A density functional theory study. Carbon, 2018, 136, 73-84.	10.3	52
20	Quantum mechanical calculation of product state distributions for the O(1D)+H2â†'OH+H reaction on the ground electronic state surface. Journal of Chemical Physics, 2000, 113, 9658-9667.	3.0	50
21	Quantum Mechanical Calculation of Reaction Probabilities and Branching Ratios for the O(1D) + HD â†' OH(OD) + D(H) Reaction on the XÌƒ1Aâ€˜and 11Aâ€˜â€˜Adiabatic Potential Energy Surfacesâ€. Journal of Physical Chemistry A, 2001, 105, 2330-2339.	2.5	50
22	The dynamics of the H⁺ + D₂reaction: a comparison of quantum mechanical wavepacket, quasi-classical and statistical-quasi-classical results. Physical Chemistry Chemical Physics, 2010, 12, 1102-1115.	2.8	48
23	DIFFREALWAVE: A parallel real wavepacket code for the quantum mechanical calculation of reactive state-to-state differential cross sections in atom plus diatom collisions. Computer Physics Communications, 2008, 179, 569-578.	7.5	43
24	Sinc wave packets: New form of wave packet for time-dependent quantum mechanical reactive scattering calculations. International Journal of Quantum Chemistry, 2003, 92, 205-211.	2.0	42
25	1D/2D C₃N₄/Graphene Composite as a Preferred Anode Material for Lithium Ion Batteries: Importance of Heterostructure Design via DFT Computation. ACS Applied Materials & Interfaces, 2020, 12, 25875-25883.	8.0	40
26	Integral and differential cross sections for the S(1D)+HD reaction employing the ground adiabatic electronic state. Physical Chemistry Chemical Physics, 2009, 11, 11587.	2.8	36
27	Improving Sensing of Sulfur-Containing Gas Molecules with ZnO Monolayers by Implanting Dopants and Defects. Journal of Physical Chemistry C, 2017, 121, 24365-24375.	3.1	35
28	Dynamics of the D+ + H2 and H+ + D2 reactions: a detailed comparison between theory and experiment. Physical Chemistry Chemical Physics, 2012, 14, 3346.	2.8	34
29	Study of the H+O2 reaction by means of quantum mechanical and statistical approaches: The dynamics on two different potential energy surfaces. Journal of Chemical Physics, 2008, 128, 244308.	3.0	32
30	Unlocking the potential of commercial carbon nanofibers as free-standing positive electrodes for flexible aluminum ion batteries. Journal of Materials Chemistry A, 2019, 7, 15123-15130.	10.3	32
31	State-to-state reaction probabilities for the H+O2(v,j)â†'O+OH(vâ€²,jâ€²) reaction on three potential energy surfaces. Journal of Chemical Physics, 2007, 127, 064316.	3.0	29
32	Exact and truncated Coriolis coupling calculations for the S(1D)+HD reaction employing the ground adiabatic electronic state. Physical Chemistry Chemical Physics, 2010, 12, 12711.	2.8	29
33	Kinetic modelling of molecular hydrogen transport in microporous carbon materials. Physical Chemistry Chemical Physics, 2011, 13, 7834.	2.8	29
34	Insights into the trapping mechanism of light metals on C2N-h2D: Utilisation as an anode material for metal ion batteries. Carbon, 2020, 160, 125-132.	10.3	29
35	Anatomy of the S(1D) + H2 reaction: the dynamics on two new potential energy surfaces from quantum dynamics calculations. Physical Chemistry Chemical Physics, 2011, 13, 13645.	2.8	26
36	Coriolis coupling effects in the dynamics of deep well reactions: application to the H+ + D2 reaction. Physical Chemistry Chemical Physics, 2011, 13, 7948.	2.8	26

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37	Three-Dimensional Silicon Carbide from Siligraphene as a High Capacity Lithium Ion Battery Anode Material. Journal of Physical Chemistry C, 2019, 123, 27295-27304.	3.1	26
38	Nonadiabatic effects in the H+H2 exchange reaction: Accurate quantum dynamics calculations at a state-to-state level. Journal of Chemical Physics, 2009, 130, 144301.	3.0	25
39	Coriolis coupling effects in the calculation of state-to-state integral and differential cross sections for the H+D2 reaction. Journal of Chemical Physics, 2007, 126, 214303.	3.0	24
40	Enriching the hydrogen storage capacity of carbon nanotube doped with polylithiated molecules. Applied Surface Science, 2018, 444, 467-473.	6.1	24
41	Functionalized carbon nitride (g-CN) monolayer as a promising energy storage material: A density functional theory study. Applied Surface Science, 2017, 419, 708-712.	6.1	22
42	Influence of Spinâ^'Orbit Effects on Chemical Reactions:â€‰ Quantum Scattering Studies for the Cl(2P) + HCl â†' ClH + Cl(2P) Reaction Using Coupled ab Initio Potential Energy Surfaces. Journal of Physical Chemistry A, 2003, 107, 7278-7289.	2.5	21
43	Quantum dynamical study of the O(D1)+HCl reaction employing three electronic state potential energy surfaces. Journal of Chemical Physics, 2008, 128, 014308.	3.0	21
44	Boosting reversible lithium storage in two-dimensional C3N4 by achieving suitable adsorption energy via Si doping. Carbon, 2021, 176, 480-487.	10.3	21
45	Graphdiyne and Hydrogen-Substituted Graphdiyne as Potential Cathode Materials for High-Capacity Aluminum-Ion Batteries. ACS Applied Energy Materials, 2020, 3, 7404-7415.	5.1	19
46	Computational Studies of the Interaction of Carbon Dioxide with Graphene-Supported Titanium Dioxide. Journal of Physical Chemistry C, 2015, 119, 29044-29051.	3.1	15
47	Doping Effects on the Performance of Paired Metal Catalysts for the Hydrogen Evolution Reaction. Journal of Chemical Information and Modeling, 2019, 59, 2242-2247.	5.4	15
48	Quantum Mechanical Calculation of Energy Dependence of OCl/OH Product Branching Ratio and Product Quantum State Distributions for the O(¹D) + HCl Reaction on All Three Contributing Electronic State Potential Energy Surfaces. Journal of Physical Chemistry A, 2008, 112, 7947-7960.	2.5	14
49	Quantum calculations for the S(1D)+H2reaction employing the ground adiabatic electronic state. Physica Scripta, 2011, 84, 028102.	2.5	14
50	Accurate prediction of binding energies for twoâ€dimensional catalytic materials using machine learning. ChemCatChem, 2020, 12, 5109-5120.	3.7	14
51	Energy dependent dynamics of the O(1D) + HCl reaction: A quantum, quasiclassical and statistical study. Physical Chemistry Chemical Physics, 2011, 13, 8502.	2.8	13
52	Significant nonadiabatic effects in the C + CH reaction dynamics. Journal of Chemical Physics, 2011, 135, 024306.	3.0	13
53	Influence of van der Waals wells on the quantum scattering dynamics of the Cl(2P)+HClâ†'ClH+Cl(2P) reaction. Chemical Physics, 2005, 308, 225-236.	1.9	12
54	Nonadiabatic quantum dynamics calculations for the N + NH â†' N2 + H reaction. Physical Chemistry Chemical Physics, 2010, 12, 9619.	2.8	12

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55	Quantum dynamics study of the N(2D)+H2 reaction and the effects of the potential energy surface on the propagation time. Computational and Theoretical Chemistry, 2012, 990, 23-29.	2.5	9
56	Nearside-farside, local angular momentum and resummation theories: Useful tools for understanding the dynamics of complex-mode reactions. AIP Advances, 2015, 5, .	1.3	9
57	Carbon nitrides as cathode materials for aluminium ion batteries. Carbon, 2021, 183, 546-559.	10.3	9
58	Quantum mechanical calculations of the S(¹D)+HD reaction dynamics on the ground electronic state. Journal of Physics: Conference Series, 2009, 185, 012056.	0.4	8
59	An accurate study of the dynamics of the C+OH reaction on the second excited 14Aâ€³ potential energy surface. Journal of Chemical Physics, 2012, 136, 164309.	3.0	8
60	Quantum Calculation of Ro-vibrational States:â€‰ Methodology and DOCl Application Results. Journal of Physical Chemistry A, 2008, 112, 4141-4147.	2.5	6
61	Interaction of Boron Nitride Nanotubes with Aluminum: A Computational Study. Journal of Physical Chemistry C, 2018, 122, 15226-15240.	3.1	6
62	A molecular dynamics model for symplectic intergrators. Mathematical Modelling of Systems, 1997, 3, 282-296.	0.7	3
63	INITIAL ROTATIONAL QUANTUM STATE EXCITATION AND ISOTOPIC EFFECTS FOR THE O(¹D)+HCl â†’ OH+Cl (OCl+H) REACTION. Journal of Theoretical and Computational Chemistry, 2009, 08, 1003-1024.	1.8	3