# Marlies Hankel

List of Publications by Year
in descending order

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|---|---|---|---|
| 63 papers | 3,341 citations | 159358 30 h-index | 143772 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. | 6.6 | 464 |
| 2 | Graphdiyne: a versatile nanomaterial for electronics and hydrogen purification. Chemical Communications, 2011, 47, 11843. | 2.2 | 329 |
| 3 | Understanding the Origin of Li<sub>2</sub>MnO<sub>3</sub> Activation in Liâ€Rich Cathode Materials for Lithiumâ€Ion Batteries. Advanced Functional Materials, 2015, 25, 7488-7496. | 7.8 | 151 |
| 4 | Evaluating the Catalytic Efficiency of Paired, Single-Atom Catalysts for the Oxygen Reduction Reaction. ACS Catalysis, 2019, 9, 7660-7667. | 5.5 | 128 |
| 5 | Enhanced CO2 photocatalytic reduction on alkali-decorated graphitic carbon nitride. Applied Catalysis B: Environmental, 2017, 216, 146-155. | 10.8 | 127 |
| 6 | Biphenylene and Phagraphene as Lithium Ion Battery Anode Materials. ACS Applied Materials & Interfaces, 2017, 9, 20577-20584. | 4.0 | 122 |
| 7 | Lithium and Sodium Storage on Graphitic Carbon Nitride. Journal of Physical Chemistry C, 2015, 119, 21921-21927. | 1.5 | 115 |
| 8 | Modelling carbon membranes for gas and isotope separation. Physical Chemistry Chemical Physics, 2013, 15, 4832. | 1.3 | 95 |
| 9 | Lithium storage on carbon nitride, graphenylene and inorganic graphenylene. Physical Chemistry Chemical Physics, 2016, 18, 14205-14215. | 1.3 | 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. | 1.2 | 85 |
| 11 | Capacitance-enhanced sodium-ion storage in nitrogen-rich hard carbon. Journal of Materials Chemistry A, 2017, 5, 22186-22192. | 5.2 | 85 |
| 12 | Asymmetrically Decorated, Doped Porous Graphene As an Effective Membrane for Hydrogen Isotope Separation. Journal of Physical Chemistry C, 2012, 116, 6672-6676. | 1.5 | 81 |
| 13 | Carbon Nitride Nanofibres with Exceptional Lithium Storage Capacity: From Theoretical Prediction to Experimental Implementation. Advanced Functional Materials, 2018, 28, 1803972. | 7.8 | 77 |
| 14 | Computational Evaluation of Lithium-Functionalized Carbon Nitride (g-C<sub>6</sub>N<sub>8</sub>) Monolayer as an Efficient Hydrogen Storage Material. Journal of Physical Chemistry C, 2016, 120, 25180-25188. | 1.5 | 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. | 9.5 | 68 |
| 16 | Sodium-intercalated bulk graphdiyne as an anode material for rechargeable batteries. Journal of Power Sources, 2017, 343, 354-363. | 4.0 | 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. | 1.5 | 65 |
| 18 | Theoretical and experimental investigations of mesoporous C3N5/MoS2 hybrid for lithium and sodium ion batteries. Nano Energy, 2020, 72, 104702. | 8.2 | 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. | 5.4 | 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. | 1.2 | 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. | 1.1 | 50 |
| 22 | The dynamics of the H<sup>+</sup> + D<sub>2</sub>reaction: a comparison of quantum mechanical wavepacket, quasi-classical and statistical-quasi-classical results. Physical Chemistry Chemical Physics, 2010, 12, 1102-1115. | 1.3 | 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. | 3.0 | 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. | 1.0 | 42 |
| 25 | 1D/2D C<sub>3</sub>N<sub>4</sub>/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. | 4.0 | 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. | 1.3 | 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. | 1.5 | 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. | 1.3 | 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. | 1.2 | 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. | 5.2 | 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. | 1.2 | 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. | 1.3 | 29 |
| 33 | Kinetic modelling of molecular hydrogen transport in microporous carbon materials. Physical Chemistry Chemical Physics, 2011, 13, 7834. | 1.3 | 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. | 5.4 | 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. | 1.3 | 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. | 1.3 | 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. | 1.5 | 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. | 1.2 | 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. | 1.2 | 24 |
| 40 | Enriching the hydrogen storage capacity of carbon nanotube doped with polylithiated molecules. Applied Surface Science, 2018, 444, 467-473. | 3.1 | 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. | 3.1 | 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. | 1.1 | 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. | 1.2 | 21 |
| 44 | Boosting reversible lithium storage in two-dimensional C3N4 by achieving suitable adsorption energy via Si doping. Carbon, 2021, 176, 480-487. | 5.4 | 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. | 2.5 | 19 |
| 46 | Computational Studies of the Interaction of Carbon Dioxide with Graphene-Supported Titanium Dioxide. Journal of Physical Chemistry C, 2015, 119, 29044-29051. | 1.5 | 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. | 2.5 | 15 |
| 48 | Quantum Mechanical Calculation of Energy Dependence of OCl/OH Product Branching Ratio and Product Quantum State Distributions for the O(<sup>1</sup>D) + HCl Reaction on All Three Contributing Electronic State Potential Energy Surfaces. Journal of Physical Chemistry A, 2008, 112, 7947-7960. | 1.1 | 14 |
| 49 | Quantum calculations for the S(1D)+H2reaction employing the ground adiabatic electronic state. Physica Scripta, 2011, 84, 028102. | 1.2 | 14 |
| 50 | Accurate prediction of binding energies for twoâ€dimensional catalytic materials using machine learning. ChemCatChem, 2020, 12, 5109-5120. | 1.8 | 14 |
| 51 | Energy dependent dynamics of the O(1D) + HCl reaction: A quantum, quasiclassical and statistical study. Physical Chemistry Chemical Physics, 2011, 13, 8502. | 1.3 | 13 |
| 52 | Significant nonadiabatic effects in the C + CH reaction dynamics. Journal of Chemical Physics, 2011, 135, 024306. | 1.2 | 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. | 0.9 | 12 |
| 54 | Nonadiabatic quantum dynamics calculations for the N + NH â†' N2 + H reaction. Physical Chemistry Chemical Physics, 2010, 12, 9619. | 1.3 | 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. | 1.1 | 9 |
| 56 | Nearside-farside, local angular momentum and resummation theories: Useful tools for understanding the dynamics of complex-mode reactions. AIP Advances, 2015, 5, . | 0.6 | 9 |
| 57 | Carbon nitrides as cathode materials for aluminium ion batteries. Carbon, 2021, 183, 546-559. | 5.4 | 9 |
| 58 | Quantum mechanical calculations of the S(<sup>1</sup>D)+HD reaction dynamics on the ground electronic state. Journal of Physics: Conference Series, 2009, 185, 012056. | 0.3 | 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. | 1.2 | 8 |
| 60 | Quantum Calculation of Ro-vibrational States:â€‰ Methodology and DOCl Application Results. Journal of Physical Chemistry A, 2008, 112, 4141-4147. | 1.1 | 6 |
| 61 | Interaction of Boron Nitride Nanotubes with Aluminum: A Computational Study. Journal of Physical Chemistry C, 2018, 122, 15226-15240. | 1.5 | 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 <font>O</font>(<sup>1</sup>D)+<font>HCl</font> â†’ <font>OH+Cl (OCl+H)</font> REACTION. Journal of Theoretical and Computational Chemistry, 2009, 08, 1003-1024. | 1.8 | 3 |