Michael Probst

List of Publications by Year
in descending order

67 papers	1,247 citations	394421 19 h-index	395702 33 g-index
67 all docs	67 docs citations	67 times ranked	1427 citing authors

#	Article	IF	Citations
1	Understanding the interactions between lithium polysulfides and anchoring materials in advanced lithiumâ€“sulfur batteries using density functional theory. Physical Chemistry Chemical Physics, 2022, 24, 8604-8623.	2.8	10
2	Sputtering and reflection from a beryllium surface: effects of hydrogen isotope mass, impact position and surface binding energy. Nuclear Fusion, 2022, 62, 066024.	3.5	2
3	Insights into glyphosate adsorption on Lewis acidic zeolites from theoretical modelling. Microporous and Mesoporous Materials, 2022, , 112083.	4.4	6
4	Electron-impact ionization cross sections of small molecules containing Fe and Cr ^{â^—}. Journal of Physics Condensed Matter, 2022, 34, 374001.	1.8	0
5	A neural network interface for DL_POLY and its application to liquid water. Molecular Simulation, 2021, 47, 113-118.	2.0	4
6	Confinement Effect on Heterogeneous Electron Transfer in Aqueous Solutions inside Conducting Nanotubes. ChemElectroChem, 2021, 8, 563-569.	3.4	7
7	Electronic structure and reactivity of tirapazamine as a radiosensitizer. Journal of Molecular Modeling, 2021, 27, 177.	1.8	2
8	Data on erosion and hydrogen fuel retention in Beryllium plasma-facing materials. Nuclear Materials and Energy, 2021, 27, 100994.	1.3	21
9	Modelling the sputtering and reflection from a beryllium surface: atomistic analysis. Nuclear Fusion, 2021, 61, 086013.	3.5	5
10	Ligand and solvent effects on the kinetics of the electrochemical reduction of Ni(II) complexes: Experiment and quantum chemical modeling. Electrochimica Acta, 2021, 395, 139138.	5.2	4
11	Halfâ€Metallic Devices from Armchair Graphene Nanoribbons with Transition Metal Guest Atoms. ChemistrySelect, 2021, 6, 347-358.	1.5	1
12	Sputtering of the beryllium tungsten alloy Be₂W by deuterium atoms: molecular dynamics simulations using machine learned forces. Nuclear Fusion, 2021, 61, 016031.	3.5	10
13	Dehydrogenation of ethanol to acetaldehyde with nitrous oxide over the metalâ€“organic framework NU-1000: a density functional theory study. Physical Chemistry Chemical Physics, 2020, 22, 13622-13628.	2.8	9
14	Iterative training set refinement enables reactive molecular dynamics via machine learned forces. RSC Advances, 2020, 10, 4293-4299.	3.6	11
15	Phenol Tautomerization Catalyzed by Acidâ€Base Pairs in Lewis Acidic Beta Zeolites: A Computational Study. ChemPhysChem, 2019, 20, 2122-2126.	2.1	5
16	Electron impact ionisation cross sections of cis- and trans-diamminedichloridoplatinum(II) and its hydrolysis products. Molecular Physics, 2019, 117, 2233-2240.	1.7	6
17	Total and partial electron impact ionization cross sections of fusion-relevant diatomic molecules. Journal of Chemical Physics, 2019, 150, 024306.	3.0	20
18	Furfural to Furfuryl Alcohol: Computational Study of the Hydrogen Transfer on Lewis Acidic BEA Zeolites and Effects of Cation Exchange and Tetravalent Metal Substitution. Inorganic Chemistry, 2018, 57, 6599-6605.	4.0	19

#	Article	IF	Citations
19	Ethane Câ€“H bond activation on the Fe(<scp>iv</scp>)â€“oxo species in a Zn-based cluster of metalâ€“organic frameworks: a density functional theory study. Physical Chemistry Chemical Physics, 2017, 19, 3782-3791.	2.8	12
20	Spin filter properties of armchair graphene nanoribbons with substitutional Fe atoms. Molecular Physics, 2017, 115, 2231-2241.	1.7	10
21	Energetics and reactivity of small beryllium deuterides. Journal of Molecular Modeling, 2017, 23, 203.	1.8	6
22	Coordinatively Unsaturated Metalâ€“Organic Frameworks M₃(btc)₂ (M = Cr, Fe,) Tj ETQq0 0 0 rgBT /Overlock Inorganic Chemistry, 2017, 56, 14005-14012.	4.0	77
23	Electron impact ionisation cross sections of iron oxides. European Physical Journal D, 2017, 71, 1.	1.3	8
24	Electron impact ionization cross sections of beryllium-tungsten clusters. European Physical Journal D, 2016, 70, 1.	1.3	11
25	Ethylene Epoxidation with Nitrous Oxide over Feâ€“BTC Metalâ€“Organic Frameworks: A DFT Study. ChemPhysChem, 2016, 17, 3416-3422.	2.1	39
26	Hydrogen Bonding and Dielectric Spectra of Ethylene Glycolâ€“Water Mixtures from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2016, 120, 10515-10523.	2.6	27
27	Electron impact ionisation cross sections of iron hydrogen clusters. European Physical Journal D, 2016, 70, 1.	1.3	7
28	Surface binding energies of beryllium/tungsten alloys. Journal of Nuclear Materials, 2016, 472, 76-81.	2.7	16
29	A DFT Study of Tungstenâ€“Methylidene Formation on a W/ZSMâ€5 Zeolite: The Metathesis Active Site. ChemPhysChem, 2015, 16, 3334-3339.	2.1	28
30	Hydration of Carbon Dioxide in Copper-Alkoxide Functionalized Metalâ€“Organic Frameworks: A DFT Study. Journal of Physical Chemistry C, 2015, 119, 3564-3571.	3.1	13
31	Vacancy patterning and patterning vacancies: controlled self-assembly of fullerenes on metal surfaces. Nanoscale, 2014, 6, 10850-10858.	5.6	6
32	Density Functional Theory Study of the Dehydrogenation of Ethanol to Acetaldehyde over the Au-Exchanged ZSM-5 Zeolite: Effect of Surface Oxygen. Journal of Physical Chemistry C, 2014, 118, 18564-18572.	3.1	22
33	Ethylene glycol revisited: Molecular dynamics simulations and visualization of the liquid and its hydrogen-bond network. Journal of Molecular Liquids, 2014, 189, 20-29.	4.9	59
34	Modeling the intrusion of molecules into graphite: Origin and shape of the barriers. International Journal of Mass Spectrometry, 2014, 365-366, 248-254.	1.5	4
35	Ordered phases of ethylene adsorbed on charged fullerenes and their aggregates. Carbon, 2014, 69, 206-220.	10.3	14
36	Electron impact ionization cross sections of beryllium and beryllium hydrides. European Physical Journal D, 2013, 67, 1.	1.3	15

#	Article	IF	Citations
37	Numerical investigation of the elastic scattering of hydrogen (isotopes) and helium at graphite (0001) surfaces at beam energies of 1 to 4ÂeV using a split-step Fourier method. Theoretical Chemistry Accounts, 2013, 132, 1337.	1.4	3
38	Interfacial Bond-Breaking Electron Transfer in Mixed Waterâ€“Ethylene Glycol Solutions: Reorganization Energy and Interplay between Different Solvent Modes. Journal of Physical Chemistry B, 2013, 117, 8793-8801.	2.6	9
39	Permeation of low-Z atoms through carbon sheets: Density functional theory study on energy barriers and deformation effects. AIP Advances, 2013, 3, 122104.	1.3	8
40	Carbonic acid revisited: Vibrational spectra, energetics and the possibility of detecting an elusive molecule. AIP Advances, 2012, 2, .	1.3	17
41	Thermal stabilization of thin gold nanowires by surfactant-coating: a molecular dynamics study. Nanoscale, 2012, 4, 585-590.	5.6	16
42	A gold cyano complex in nitromethane: MD simulation and X-ray diffraction. Chemical Physics Letters, 2012, 539-540, 24-29.	2.6	0
43	Au(CN)2(CH3NO2)n cluster anions: Energetics and geometrical features. Journal of Molecular Liquids, 2011, 159, 38-41.	4.9	2
44	Inside Cover: Oxidative Dehydrogenation of Propane over a VO2-Exchanged MCM-22 Zeolite: A DFT Study (ChemPhysChem 16/2010). ChemPhysChem, 2010, 11, 3370-3370.	2.1	0
45	Adsorption and Tautomerization Reaction of Acetone on Acidic Zeolites: The Confinement Effect in Different Types of Zeolites. Journal of Physical Chemistry C, 2010, 114, 15061-15067.	3.1	62
46	Potential energy surface and molecular dynamics simulation of gold(I) in liquid nitromethane. Journal of Molecular Liquids, 2009, 147, 64-70.	4.9	2
47	Chapter 3 The Semiempirical Deutschâ€“MÃrk Formalism. Advances in Atomic, Molecular and Optical Physics, 2009, 57, 87-155.	2.3	19
48	CALCULATION OF PROCESSES RELEVANT TO REACTIONS BETWEEN NUCLEIC ACIDS AND FREE ELECTRONS. Chemical Engineering Communications, 2008, 195, 1371-1381.	2.6	1
49	Medium and Interfacial Effects in the Multistep Reduction of Binuclear Complexes with Robson-Type Ligand. Inorganic Chemistry, 2008, 47, 6659-6673.	4.0	9
50	Mass Spectrometric Investigation of Anions Formed upon Free Electron Attachment to Nucleobase Molecules and Clusters Embedded in Superfluid Helium Droplets. Physical Review Letters, 2006, 97, 043201.	7.8	94
51	Polarization damping in halideâ€“water dimers. Chemical Physics Letters, 2006, 420, 267-270.	2.6	27
52	Structural investigation of lithium iodide in liquid dimethyl sulfoxide: Comparison between experiment and computation. Chemical Physics, 2006, 321, 100-110.	1.9	19
53	Structure and adsorption of a basic probe molecule on H-ZSM-5 nanostructured zeolite: An embedded ONIOM study. Journal of Molecular Graphics and Modelling, 2006, 25, 219-225.	2.4	33
54	Computational study of hydrated phosphate anions. Journal of Molecular Liquids, 2005, 118, 15-25.	4.9	39

#	Article	IF	Citations
55	Molecular dynamics simulation of lithium iodide in liquid dimethylsulfoxide. Chemical Physics Letters, 2005, 401, 217-222.	2.6	17
56	On the performance of molecular polarization methods close to a point charge. Computer Physics Communications, 2005, 169, 331-334.	7.5	6
57	Pyridine adsorbed on H-Faujasite zeolite: Electrostatic effect of the infinite crystal lattice calculated from a point charge representation. International Journal of Quantum Chemistry, 2005, 105, 898-905.	2.0	20
58	On the performance of molecular polarization methods. II. Water and carbon tetrachloride close to a cation. Journal of Chemical Physics, 2005, 123, 164505.	3.0	58
59	Comparison of methods for point-charge representation of electrostatic fields. International Journal of Quantum Chemistry, 2004, 96, 17-22.	2.0	12
60	On the performance of molecular polarization methods. I. Water and carbon tetrachloride close to a point charge. Journal of Chemical Physics, 2004, 121, 7362-7378.	3.0	38
61	X-ray and neutron diffraction studies and molecular dynamics simulations of liquid DMSO. Physical Chemistry Chemical Physics, 2004, 6, 2136-2144.	2.8	34
62	Ab initio study of the interaction of dimethylsulfoxide with the ions Li+ and Iâˆ’. International Journal of Mass Spectrometry, 2003, 223-224, 263-270.	1.5	6
63	Molecular dynamics study of an aqueous potassium nitrate solution. International Journal of Quantum Chemistry, 1999, 75, 805-814.	2.0	21
64	Quantum chemical study of the interaction of nitrate anion with water. International Journal of Quantum Chemistry, 1998, 70, 877-886.	2.0	29
65	Representation of Intermolecular Potential Functions by Neural Networks. Journal of Physical Chemistry A, 1998, 102, 4596-4605.	2.5	105
66	Correlation between intramolecular bond distances and stretching vibrations for polar molecules: An ab initio study. International Journal of Quantum Chemistry, 1997, 63, 537-546.	2.0	7
67	Quantum chemical study of the molecular dynamics of hydrated Li+ And Be2+ cations. International Journal of Quantum Chemistry, 1997, 65, 803-816.	2.0	18