Bernd Hartke

List of Publications by Year
in descending order

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113	3,991	109137	133063
papers	citations	35 h-index	59 g-index

127	127	127	2831
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Globally Optimized Molecular Embeddings for Dynamic Reaction Solvate Shell Optimization and Active Site Design. Topics in Catalysis, 2022, 65, 281-288.	1.3	4
2	Implicitly perturbed Hamiltonian as a class of versatile and general-purpose molecular representations for machine learning. Nature Communications, 2022, 13, 1245.	5.8	1
3	Electrooxidation of Alcohols on Mixed Copperâ€“Cobalt Hydroxycarbonates in Alkaline Solution. ChemElectroChem, 2022, 9, .	1.7	6
4	SIMULATION OF MOLECULAR MACHINES. , 2021, , .		0
5	Improved prediction of solvation free energies by machine-learning polarizable continuum solvation model. Nature Communications, 2021, 12, 3584.	5.8	46
6	Disordered Two-Dimensional Self-Organization of Ethyl Pyruvate Molecules on the Pt(111) Surface. Journal of Physical Chemistry C, 2021, 125, 26167-26179.	1.5	4
7	The Impact of Electronic Effects on Photolysis: A Model Study on the 4,5â€Dimethoxyâ€2â€nitrobenzyl Caged Nâ€Phenylpyrimidineâ€2â€amine Scaffold. ChemPhotoChem, 2020, 4, 638-643.	1.5	5
8	Globally optimal catalytic fields for a Dielsâ€“Alder reaction. Journal of Chemical Physics, 2020, 152, 114106.	1.2	21
9	Full-Dimensional Photodynamics of Bistable Proton Transfer Switches. Zeitschrift Fur Physikalische Chemie, 2020, 234, 1533-1547.	1.4	3
10	Tuning the Strength of Molecular Bonds in Oxygenates via Surface-Assisted Intermolecular Interactions: Atomistic Insights. Journal of Physical Chemistry C, 2020, 124, 28159-28168.	1.5	9
11	Exploring selfâ€organization of molecular tether molecules on a gold surface by global structure optimization. Journal of Computational Chemistry, 2019, 40, 1978-1989.	1.5	8
12	Malleable parallelism with minimal effort for maximal throughput and maximal hardware load. Computational and Theoretical Chemistry, 2019, 1151, 72-77.	1.1	4
13	Simulations of optically switchable molecular machines for particle transport. Journal of Computational Chemistry, 2018, 39, 1433-1443.	1.5	4
14	Future Perspectives: Using Computer Simulations to Supplement Studentsâ€™ Introduction to Scientific Inquiry. Chemkon - Chemie Konkret, Forum Fuer Unterricht Und Didaktik, 2018, 25, 285-292.	0.2	0
15	Axitinib: A Photoswitchable Approved Tyrosine Kinase Inhibitor. ChemMedChem, 2018, 13, 2415-2426.	1.6	34
16	Cluster structures influenced by interaction with a surface. Physical Chemistry Chemical Physics, 2018, 20, 15661-15670.	1.3	6
17	Resonance dynamics of DCO (X̃ƒâ€‰Aâ€²2) simulated with the dynamically pruned discrete variable representation (DP-DVR). Journal of Chemical Physics, 2018, 148, 204309.	1.2	4
18	Globally Optimal Catalytic Fields â€“ Inverse Design of Abstract Embeddings for Maximum Reaction Rate Acceleration. Journal of Chemical Theory and Computation, 2018, 14, 3547-3564.	2.3	29

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19	Cheap but accurate calculation of chemical reaction rate constants from ab initio data, via system-specific, black-box force fields. Journal of Chemical Physics, 2017, 147, 161701.	1.2	8
20	Full-Dimensional Excited-State Intramolecular Proton Transfer Dynamics of Salicylic Acid. Journal of Physical Chemistry A, 2017, 121, 5967-5977.	1.1	15
21	Ultrafast dynamics of UV-excited trans- and cis-ferulic acid in aqueous solutions. Physical Chemistry Chemical Physics, 2017, 19, 30683-30694.	1.3	20
22	Conquering the hard cases of Lennard-Jones clusters with simple recipes. Computational and Theoretical Chemistry, 2017, 1107, 7-13.	1.1	20
23	Improved Cluster Structure Optimization: Hybridizing Evolutionary Algorithms with Local Heat Pulses. Inorganics, 2017, 5, 64.	1.2	9
24	Efficient molecular quantum dynamics in coordinate and phase space using pruned bases. Journal of Chemical Physics, 2016, 145, 204108.	1.2	32
25	Error-Safe, Portable, and Efficient Evolutionary Algorithms Implementation with High Scalability. Journal of Chemical Theory and Computation, 2016, 12, 5226-5233.	2.3	11
26	<scp>reax</scp>FF Reactive Force Field for Disulfide Mechanochemistry, Fitted to Multireference ab Initio Data. Journal of Chemical Theory and Computation, 2016, 12, 3913-3925.	2.3	28
27	Efficient global optimization of reactive forceâ€field parameters. Journal of Computational Chemistry, 2015, 36, 1550-1561.	1.5	51
28	Lokalisierung eines mechanochemischen Bindungsbruchs durch Einbettung des Mechanophors in einen Makrocyclus. Angewandte Chemie, 2015, 127, 2587-2590.	1.6	14
29	Reactive force fields made simple. Physical Chemistry Chemical Physics, 2015, 17, 16715-16718.	1.3	29
30	Pinpointing Mechanochemical Bond Rupture by Embedding the Mechanophore into a Macrocycle. Angewandte Chemie - International Edition, 2015, 54, 2556-2559.	7.2	47
31	Observable-targeting global cluster structure optimization. Physical Chemistry Chemical Physics, 2015, 17, 11958-11961.	1.3	9
32	Indandiazocines: unidirectional molecular switches. ScienceOpen Research, 2015, .	0.6	2
33	A graphâ€based shortâ€cut to lowâ€energy structures. Journal of Computational Chemistry, 2014, 35, 1618-1620.	1.5	9
34	Photochemical dynamics of E-methylfurylfulgideâ€”kinematic effects on photorelaxation dynamics of furylfulgides. Physical Chemistry Chemical Physics, 2014, 16, 2483-2490.	1.3	19
35	A size resolved investigation of large water clusters. Physical Chemistry Chemical Physics, 2014, 16, 6859.	1.3	91
36	Computerâ€Assisted Synthesis Optimisation of Inorganicâ€“Organic Hybrid Compounds Using the Local Optimisation Algorithm BOBYQA. ChemPlusChem, 2014, 79, 863-871.	1.3	6

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37	Assessing Solvation Effects on Chemical Reactions with Globally Optimized Solvent Clusters. ChemPhysChem, 2013, 14, 2678-2686.	1.0	10
38	Global optimization of parameters in the reactive force field ReaxFF for SiOH. Journal of Computational Chemistry, 2013, 34, 2178-2189.	1.5	77
39	Photochemical properties of multi-azobenzene compounds. Photochemical and Photobiological Sciences, 2013, 12, 511-518.	1.6	45
40	Importance of a low-lying nÏ€*-state in the photo-isomerisation reaction of Z-methylfurylfulgide. Journal of Photochemistry and Photobiology A: Chemistry, 2013, 263, 34-40.	2.0	6
41	Approximate photochemical dynamics of azobenzene with reactive force fields. Journal of Chemical Physics, 2013, 139, 224303.	1.2	21
42	Photochemical dynamics of E-iPr-furylfulgide. Physical Chemistry Chemical Physics, 2012, 14, 12193.	1.3	27
43	Simulating a Molecular Machine in Action. Journal of Physical Chemistry A, 2012, 116, 11241-11248.	1.1	10
44	Empirical Review of Standard Benchmark Functions Using Evolutionary Global Optimization. Applied Mathematics, 2012, 03, 1552-1564.	0.1	76
45	Design of optimally switchable molecules by genetic algorithms. Physical Chemistry Chemical Physics, 2011, 13, 2903-2910.	1.3	23
46	Superior Z â†' E and E â†' Z photoswitching dynamics of dihydrodibenzodiazocine, a bridged azobenzene, by S₁(nÏ€*) excitation at Î» = 387 and 490 nm. Physical Chemistry Chemical Physics, 2011, 13, 1054-1063.	1.3	86
47	Global optimization. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 879-887.	6.2	72
48	Aggregation of Kanamycin A: dimer formation with physiological cations. Journal of Molecular Modeling, 2011, 17, 3195-3207.	0.8	13
49	Compositionâ€induced structural transitions in mixed Lennardâ€Jones clusters: Global reparametrization and optimization. Journal of Computational Chemistry, 2011, 32, 1377-1385.	1.5	50
50	Towards automated multi-dimensional quantum dynamical investigations of double-minimum potentials: Principles and example applications. Chemical Physics, 2011, 380, 1-8.	0.9	5
51	Unusual photochemical dynamics of a bridged azobenzene derivative. Journal of Chemical Physics, 2010, 133, 124305.	1.2	52
52	Photochemical Ring-Opening of Cyclohexadiene: Quantum Wavepacket Dynamics on a Global Ab Initio Potential Energy Surface. Journal of Physical Chemistry A, 2010, 114, 4036-4044.	1.1	33
53	OGOLEM: Global cluster structure optimisation for arbitrary mixtures of flexible molecules. A multiscaling, object-oriented approach. Molecular Physics, 2010, 108, 279-291.	0.8	101
54	Brownian molecular rotors: Theoretical design principles and predicted realizations. Journal of Chemical Physics, 2009, 130, 234906.	1.2	10

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55	Methane-water clusters under pressure: Are clathrate cages optimal clusters?. Journal of Chemical Physics, 2009, 130, 024905.	1.2	12
56	Modeling of high-order many-mode terms in the expansion of multidimensional potential energy surfaces: Application to vibrational spectra. Journal of Chemical Physics, 2009, 131, 014108.	1.2	32
57	Quantum-mechanical wavepacket propagation in a sparse, adaptive basis of interpolating Gaussians with collocation. Physical Chemistry Chemical Physics, 2009, 11, 463-475.	1.3	28
58	Morphing Lennardâ€"Jones clusters to TIP4P water clusters: Why do water clusters look like they do?. Chemical Physics, 2008, 346, 286-294.	0.9	11
59	Structural Correspondences between the Low-Energy Nanoclusters of Silica and Water. Journal of Physical Chemistry C, 2008, 112, 18417-18425.	1.5	7
60	Differential effects of oligosaccharides on the hydration of simple cations. Journal of Chemical Physics, 2008, 128, 105105.	1.2	15
61	Links between potential energy structures and quantum cumulative reaction probabilities of double proton transfer reactions. Chemical Physics, 2007, 338, 160-167.	0.9	5
62	Propagation with distributed Gaussians as a sparse, adaptive basis for higher-dimensional quantum dynamics. Physical Chemistry Chemical Physics, 2006, 8, 3627.	1.3	28
63	Fingerprints of Delocalized Transition States in Quantum Dynamics. Journal of Physical Chemistry A, 2006, 110, 13014-13021.	1.1	14
64	Larger Water Clusters with Edges and Corners on Their Way to Ice:Â Structural Trends Elucidated with an Improved Parallel Evolutionary Algorithm. Journal of Physical Chemistry A, 2006, 110, 5809-5822.	1.1	106
65	Inhalte statt Verpackung. Nachrichten Aus Der Chemie, 2006, 54, 1181-1181.	0.0	0
66	A contribution to the structure of the van-der-Waals complex phenylacetyleneâ€"argon by microwave spectroscopy and quantum chemistry. Journal of Molecular Structure, 2006, 825, 1-19.	1.8	10
67	Efficient Global Geometry Optimization of Atomic and Molecular Clusters. , 2006, , 141-168.		7
68	Towards protein folding with evolutionary techniques. Journal of Computational Chemistry, 2005, 26, 1169-1179.	1.5	20
69	A new proposal for the reason of magic numbers in alkali cation microhydration clusters. Theoretical Chemistry Accounts, 2005, 114, 357-379.	0.5	27
70	GLOBAL GEOMETRY OPTIMIZATION OF SILICON CLUSTERS EMPLOYING EMPIRICAL POTENTIALS, DENSITY FUNCTIONALS, AND AB INITIO CALCULATIONS. Journal of Theoretical and Computational Chemistry, 2005, 04, 1119-1151.	1.8	13
71	Double proton transfer reactions at the transition from a concerted to a stepwise mechanism: a comparative ab initio study. Physical Chemistry Chemical Physics, 2005, 7, 493.	1.3	18
72	A contribution to the microwave spectrum and structure of phenylacetylene. Journal of Molecular Structure, 2004, 698, 1-24.	1.8	20

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73	Global and local optimization of auxiliary basis sets for RI-MP2 calculations. Physical Chemistry Chemical Physics, 2004, 6, 5456.	1.3	14
74	Analysis and dynamics of unusual double proton transfer reactions based on the reaction path Hamiltonian. Physical Chemistry Chemical Physics, 2004, 6, 3341.	1.3	13
75	Global geometry optimization of small silicon clusters with empirical potentials and at the DFT level. Physical Chemistry Chemical Physics, 2004, 6, 503.	1.3	46
76	Efficient global geometry optimization of clusters. European Physical Journal D, 2003, 24, 57-60.	0.6	19
77	Structural information on alkali cation microhydration clusters from infrared spectra. Physical Chemistry Chemical Physics, 2003, 5, 5021.	1.3	35
78	Size-dependent transition from all-surface to interior-molecule structures in pure neutral water clusters. Physical Chemistry Chemical Physics, 2003, 5, 275-284.	1.3	96
79	Structural Trends and Transitions in Water Clusters. , 2003, , 205-214.		0
80	Theoretische Chemie 2001. Nachrichten Aus Der Chemie, 2002, 50, 327-335.	0.0	0
81	Experimental and theoretical investigation of microsolvation of Na+-ions in the gas phase by high resolution mass spectrometry and global cluster geometry optimization. Journal of Chemical Physics, 2002, 116, 3588-3600.	1.2	54
82	StrukturÃ¼bergÃnge in Clustern. Angewandte Chemie, 2002, 114, 1534-1554.	1.6	12
83	Structural Transitions in Clusters. Angewandte Chemie - International Edition, 2002, 41, 1468-1487.	7.2	117
84	Dodecahedral Clathrate Structures and Magic Numbers in Alkali Cation Microhydration Clusters. ChemPhysChem, 2002, 3, 98-106.	1.0	59
85	Structures of mercury clusters in a quantumâ€“empirical hybrid model. Physical Chemistry Chemical Physics, 2001, 3, 5121-5129.	1.3	31
86	Calculation of the Raman Spectrum of Photodissociating H2S around 195 nmâ€. Journal of Physical Chemistry A, 2001, 105, 2458-2467.	1.1	7
87	Global Geometry Optimization of Molecular Clusters: TIP4P Water. Zeitschrift Fur Physikalische Chemie, 2000, 214, .	1.4	55
88	Global cluster geometry optimization by a phenotype algorithm with Niches: Location of elusive minima, and low-order scaling with cluster size. Journal of Computational Chemistry, 1999, 20, 1752-1759.	1.5	178
89	Photodissociation dynamics of H2S on new coupled ab initio potential energy surfaces. Journal of Chemical Physics, 1999, 111, 4523-4534.	1.2	159
90	Global geometry optimization of small silicon clusters at the level of density functional theory. Theoretical Chemistry Accounts, 1998, 99, 241-247.	0.5	43

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91	Improved intermolecular water potential from global geometry optimization of small water clusters using local MP2. Chemical Physics, 1998, 239, 561-572.	0.9	51
92	Quantum mechanical and quasiclassical simulations of molecular beam experiments for the F+H2â†'HF+H reaction on two ab initio potential energy surfaces. Journal of Chemical Physics, 1998, 109, 7224-7237.	1.2	81
93	Time-dependent quantum simulations of FH2â¯ photoelectron spectra on new ab initio potential energy surfaces for the anionic and the neutral species. Chemical Physics Letters, 1997, 280, 430-438.	1.2	77
94	Global geometry optimization of clusters guided by N-dependent model potentials. Chemical Physics Letters, 1996, 258, 144-148.	1.2	55
95	Global geometry optimization of (Ar)n and B(Ar)n clusters using a modified genetic algorithm. Journal of Chemical Physics, 1996, 104, 2684-2691.	1.2	123
96	Global geometry optimization of clusters using a growth strategy optimized by a genetic algorithm. Chemical Physics Letters, 1995, 240, 560-565.	1.2	45
97	Ab initio molecular dynamics simulated annealing at the generalized valence bond level. Application to a small nickel cluster. Chemical Physics Letters, 1993, 216, 324-328.	1.2	27
98	Multiple time scale Hartree-Fock molecular dynamics. International Journal of Quantum Chemistry, 1993, 45, 59-70.	1.0	30
99	Global geometry optimization of clusters using genetic algorithms. The Journal of Physical Chemistry, 1993, 97, 9973-9976.	2.9	258
100	Scattering delay times and transition rates for continuum resonance Raman scattering: Detailed derivations via the timeâ€dependent approach and applications to 79Br2. Journal of Chemical Physics, 1992, 96, 5636-5649.	1.2	20
101	Ab initio molecular dynamics with correlated molecular wave functions: Generalized valence bond molecular dynamics and simulated annealing. Journal of Chemical Physics, 1992, 97, 6569-6578.	1.2	115
102	Local versus hyperspherical modes of water and formaldehyde: Effect of molecular complexity on modeâ€selective structures and dynamics. Journal of Chemical Physics, 1992, 96, 3569-3584.	1.2	15
103	Spin eigenstate-dependent Hartreeâ€"Fock molecular dynamics. Chemical Physics Letters, 1992, 189, 358-362.	1.2	106
104	Connecting level statistics and reaction dynamics: Mode selective decay of resonant states for HXXH-type molecules. Chemical Physics, 1991, 154, 63-84.	0.9	4
105	Continuum resonance Raman scattering in bromine: Comparison of time-dependent calculations with time-independent and experimental results. Journal of Raman Spectroscopy, 1991, 22, 131-140.	1.2	21
106	Model Calculations on Laser Induced Dissociation of Bromine with Control of Electronic Product Excitation. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1990, 94, 1312-1318.	0.9	19
107	Quantum simulation of femtosecond population control in iodine. Chemical Physics Letters, 1990, 175, 322-326.	1.2	10
108	Continuum resonance Raman scattering in diatomic molecules: Experiment and theory. Vibrational Spectroscopy, 1990, 1, 119-124.	1.2	14

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109	A new quantum isotope effect: Extreme local mode selectivity in unimolecular dissociations imposed by antagonism between dynamic propensities of educts and zero point energies of products. Journal of Chemical Physics, 1990, 92, 220-226.	1.2	12
110	Large amplitude ground state vibrational coherence induced by impulsive absorption in CsI. A computer simulation. Chemical Physics Letters, 1989, 158, 238-244.	1.2	87
111	Sensitivity of resonance Raman spectra to changes in the potential: A time-dependent approach. Chemical Physics Letters, 1989, 160, 538-542.	1.2	26
112	Mode selective control of unimolecular dissociations: Survey, and model simulations for HDO â† H+DO, D+HO. Chemical Physics, 1989, 139, 123-146.	0.9	61
113	Do chemical reactions react along the reaction path?. Journal of the American Chemical Society, 1988, 110, 3063-3068.	6.6	32