Dunyou Wang

List of Publications by Year
in descending order

71 papers	6,492 citations	279798 23 h-index	102487 66 g-index
71 all docs	71 docs citations	71 times ranked	10491 citing authors

#	Article	IF	Citations
1	Theoretical dynamics studies of the CH₃ + HBr â†' CH₄ + Br reaction: integral cross sections, rate constants and microscopic mechanism. Physical Chemistry Chemical Physics, 2022, , .	2.8	6
2	Theoretical investigation of the S_N2 mechanism of X^{â^'} [X = SH, PH₂] + CH₃Y [Y = F, Cl, Br, I] reactions in water. Physical Chemistry Chemical Physics, 2021, 23, 23267-23273.	2.8	4
3	Catalytic Descriptors to Investigate Catalytic Power in the Reaction of Haloalkane Dehalogenase Enzyme with 1,2-Dichloroethane. International Journal of Molecular Sciences, 2021, 22, 5854.	4.1	0
4	Using quantum dynamics to study the effect of energy efficiency on the reactivity of the OH + DBr reaction. Physical Chemistry Chemical Physics, 2021, 23, 24669-24676.	2.8	0
5	Predicting atomic-level reaction mechanisms for SN2 reactions via machine learning. Journal of Chemical Physics, 2021, 155, 224111.	3.0	2
6	Time-dependent quantum dynamics study of the F + C₂H₆ â†' HF + C₂H₅ reaction. Physical Chemistry Chemical Physics, 2021, 23, 26911-26918.	2.8	6
7	Quantum dynamics study of isotope effects of the OD/OHâ€‰+â€‰CH3 reactions. Molecular Physics, 2020, 118, e1710610.	1.7	0
8	Multilevel Quantum Mechanics and Molecular Mechanics Study of the Double-Inversion Mechanism at Nitrogen: F^{â€“} + NH₂Cl in Aqueous Solution. Journal of Physical Chemistry A, 2020, 124, 141-147.	2.5	7
9	Methanol synthesis from CO2/H2 on Cu (1â€¯0â€¯0): Two-tier ab initio molecular dynamics study. Applied Surface Science, 2020, 505, 144528.	6.1	5
10	Oscillating collective motion of active rotors in confinement. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 11901-11907.	7.1	44
11	The importance of the composite mechanisms with two transition states in the F^{â^'} + NH₂I S_N2 reaction. Physical Chemistry Chemical Physics, 2020, 22, 12929-12938.	2.8	13
12	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	3.0	425
13	Hybrid Solvation Model with First Solvation Shell for Calculation of Solvation Free Energy. ChemPhysChem, 2020, 21, 762-769.	2.1	5
14	Quantum dynamics study of kinetic isotope effects of OD with HBr and DBr. Physical Chemistry Chemical Physics, 2019, 21, 14722-14727.	2.8	3
15	Controlling the conductance of single-molecule junctions with high spin filtering efficiency by intramolecular proton transfer. Organic Electronics, 2019, 64, 7-14.	2.6	12
16	Catalytic Effect of Aqueous Solution in Water-Assisted Proton-Transfer Mechanism of 8-Hydroxy Guanine Radical. Journal of Physical Chemistry B, 2018, 122, 3124-3132.	2.6	5
17	Solvent effects and potential of mean force study of the S _N 2 reaction of CH ₃ +CN ^{â^'} in water. Chinese Physics B, 2018, 27, 033401.	1.4	5
18	Newly proposed proton-abstraction roundabout with backside attack mechanism for the S_N2 reaction at the nitrogen center in F^{â^'} + NH₂Cl. Physical Chemistry Chemical Physics, 2018, 20, 12106-12111.	2.8	10

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19	Fabricating Atom-Sized Gaps by Field-Aided Atom Migration in Nanoscale Junctions. Physical Review Applied, 2018, 9, .	3.8	31
20	Quantum dynamics calculations reveal temperature independence of kinetic isotope effect of the OH + HBr/DBr reaction. Journal of Chemical Physics, 2018, 149, 034302.	3.0	5
21	Quantum dynamics study of energy requirement on reactivity for the HBrâ€‰+â€‰OH reaction with a negative-energy barrier. Scientific Reports, 2017, 7, 40314.	3.3	8
22	Multi-level quantum mechanics theories and molecular mechanics study of the double-inversion mechanism of the F^{â˜’}+ CH₃I reaction in aqueous solution. Physical Chemistry Chemical Physics, 2017, 19, 14358-14365.	2.8	18
23	Quantum Dynamics Study of the Potential Energy Minima Effect on Energy Efficiency for the Fâ€“ + CH3Cl â†’ FCH3 + Clâ€“ Reaction. Journal of Physical Chemistry A, 2017, 121, 2773-2779.	2.5	14
24	Multilevel Quantum Mechanics Theories and Molecular Mechanics Calculations of the Cl^{â€“} + CH₃I Reaction in Water. Journal of Physical Chemistry A, 2017, 121, 8012-8016.	2.5	3
25	Multi-level Quantum Mechanics and Molecular Mechanics Study of Ring Opening Process of Guanine Damage by Hydroxyl Radical in Aqueous Solution. Scientific Reports, 2017, 7, 7798.	3.3	5
26	Combined multi-level quantum mechanics theories and molecular mechanics study of water-induced transition state of OH ^{â˜’} +CO ₂ reaction in aqueous solution. Chinese Physics B, 2017, 26, 103401.	1.4	0
27	The effects of proportion and location of pyrimidinyl for modulation of rectification on the structure of quaterphenyl. Chemical Physics Letters, 2016, 666, 38-44.	2.6	0
28	A new, double-inversion mechanism of the F^{â˜’} + CH₃Cl S_N2 reaction in aqueous solution. Physical Chemistry Chemical Physics, 2016, 18, 31895-31903.	2.8	32
29	A multi-level quantum mechanics and molecular mechanics study of S_N2 reaction at nitrogen: NH₂Cl + OH^{â˜’}in aqueous solution. Physical Chemistry Chemical Physics, 2016, 18, 6146-6152.	2.8	11
30	Investigation of the CH3Cl + CNâ˜’ reaction in water: Multilevel quantum mechanics/molecular mechanics study. Journal of Chemical Physics, 2015, 142, 244505.	3.0	17
31	Ab Initio Study of Guanine Damage by Hydroxyl Radical. Journal of Physical Chemistry A, 2015, 119, 377-382.	2.5	12
32	Quantum mechanical and molecular mechanics approach with a multilayered-quantum representation study of solvent effects and potentials of mean force for the CH3CH2ClÂ+ÂClOâ˜’ SN2 reaction in aqueous solution. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	1
33	Energy efficiency in surmounting the central energy barrier: a quantum dynamics study of the OH + CH₃ â†’ O + CH₄ reaction. Physical Chemistry Chemical Physics, 2015, 17, 5187-5193.	2.8	13
34	A seven-degree-of-freedom, time-dependent quantum dynamics study on the energy efficiency in surmounting the central energy barrier of the OH + CH3 â†’ O + CH4 reaction. Journal of Chemical Physics, 2015, 142, 164303.	3.0	15
35	Quantum dynamics study of energy efficiency on reactivity for the double-barrier potential energy surface of the N+N2 reaction. Chemical Physics Letters, 2015, 633, 202-207.	2.6	5
36	Solvent effects and potential of mean force: a multilayered-representation quantum mechanical/molecular mechanics study of the CH₃Br + CN^{â˜’} reaction in aqueous solution. Physical Chemistry Chemical Physics, 2014, 16, 19993-20000.	2.8	11

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37	A multilayered-representation, quantum mechanical/molecular mechanics study of the CH₃Cl + F^{â˙} reaction in aqueous solution: the reaction mechanism, solvent effects and potential of mean force. Physical Chemistry Chemical Physics, 2014, 16, 7611-7617.	2.8	20
38	A multilayered representation, quantum mechanical and molecular mechanics study of the CH₃Fâ€‰+â€‰OH^{â˙} reaction in water. Journal of Computational Chemistry, 2014, 35, 445-450.	3.3	13
39	Quantum reaction dynamics study of vibrational excitation effects on the Cl+CHD3/CD4â†'HCl/DCl+CD3 reactions. Chemical Physics Letters, 2014, 603, 41-45.	2.6	6
40	Water assisted reaction mechanism of OHâ˙ with CCl4 in aqueous solution â€“ Hybrid quantum mechanical and molecular mechanics investigation. Chemical Physics Letters, 2013, 559, 30-34.	2.6	5
41	Quantum Dynamics Study of the F + CH₄ â†' HF + CH₃ Reaction on an Ab Initio Potential Energy Surface. Journal of Physical Chemistry A, 2013, 117, 7124-7130.	2.5	30
42	Quantum Dynamics Study of Vibrational Excitation Effects and Energy Requirement on Reactivity for the O + CD₄/CHD₃ â†' OD/OH + CD₃ Reactions. Journal of Physical Chemistry A, 2013, 117, 12236-12242.	2.5	23
43	A multilayered-representation quantum mechanical/molecular mechanics study of the SN2 reaction of CH3Br + OHâ˙ in aqueous solution. Journal of Chemical Physics, 2012, 137, 184501.	3.0	19
44	Quantum dynamics study of the Cl + CH4 â†' HCl + CH3 reaction: reactive resonance, vibrational excitation reactivity, and rate constants. Physical Chemistry Chemical Physics, 2012, 14, 13656.	2.8	42
45	Hybrid Quantum Mechanical and Molecular Mechanics Study of the S_N2 Reaction of CCl₄ + OH^{â€“} in Aqueous Solution: The Potential of Mean Force, Reaction Energetics, and Rate Constants. Journal of Physical Chemistry A, 2012, 116, 2371-2376.	2.5	26
46	CH₂Cl₂ + OH^{â˙} Reaction in Aqueous Solution: A Combined Quantum Mechanical and Molecular Mechanics Study. Journal of Physical Chemistry A, 2011, 115, 1380-1384.	2.5	13
47	Hybrid Quantum Mechanical/Molecular Mechanics Study of the S_N2 Reaction of CH₃Cl+OH^{â€“} in Water. Journal of Physical Chemistry A, 2011, 115, 12047-12052.	2.5	41
48	A quantum reaction dynamics study of the translational, vibrational, and rotational motion effects on the HD + ${m H}_3^+$H3+ reaction. Journal of Chemical Physics, 2011, 135, 114307.	3.0	3
49	Some insights into mechanism for binding and drug resistance of wild type and I50V V82A and I84V mutations in HIV-1 protease with GRL-98065 inhibitor from molecular dynamic simulations. European Journal of Medicinal Chemistry, 2010, 45, 227-235.	5.5	30
50	NWChem: A comprehensive and scalable open-source solution for large scale molecular simulations. Computer Physics Communications, 2010, 181, 1477-1489.	7.5	4,740
51	Eight-dimensional, quantum reaction dynamics, study of the isotopic reaction D2+C2H. Chemical Physics Letters, 2010, 490, 4-8.	2.6	4
52	Seven-degree-of-freedom, quantum scattering dynamics study of the H2D++H2 reaction. Journal of Chemical Physics, 2010, 132, 084305.	3.0	9
53	An eight-degree-of-freedom quantum dynamics study of the isotopic effect on the reaction: HD+C2H. Journal of Chemical Physics, 2008, 129, 084303.	3.0	14
54	An eight-degree-of-freedom, time-dependent quantum dynamics study for the H2+C2H reaction on a new modified potential energy surface. Journal of Chemical Physics, 2007, 127, 154304.	3.0	11

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55	A full dimensional, nine-degree-of-freedom, time-dependent quantum dynamics study for the H2+C2H reaction. Journal of Chemical Physics, 2006, 124, 201105.	3.0	41
56	An eight-degree-of-freedom quantum dynamics study for the H2+C2H system. Journal of Chemical Physics, 2005, 123, 194302.	3.0	28
57	Quantum study of the N+N2 exchange reaction: State-to-state reaction probabilities, initial state selected probabilities, Feshbach resonances, and product distributions. Journal of Chemical Physics, 2004, 120, 6041-6050.	3.0	34
58	Reactive resonances in the N+N2 exchange reaction. Chemical Physics Letters, 2003, 379, 132-138.	2.6	23
59	Quantal study of the exchange reaction for N+N2 using an ab initio potential energy surface. Journal of Chemical Physics, 2003, 118, 2186-2189.	3.0	74
60	Quantum dynamics study of the isotopic effect on capture reactions: HD, D2+CH3. Journal of Chemical Physics, 2003, 118, 1184-1188.	3.0	24
61	Quantum dynamics scattering study of AB+CDE reactions: A seven-dimensional treatment for the H2+C2H reaction. Journal of Chemical Physics, 2003, 119, 12057-12062.	3.0	24
62	Resonances in the O(3P)+HCl reaction due to van der Waals minima. Journal of Chemical Physics, 2002, 116, 7461-7467.	3.0	59
63	A time-dependent quantum dynamics study of the H2+CH3â†'H+CH4 reaction. Journal of Chemical Physics, 2002, 117, 9806-9810.	3.0	33
64	A reduced dimensionality, six-degree-of-freedom, quantum calculation of the H+CH4â†'H2+CH3 reaction. Journal of Chemical Physics, 2001, 115, 2055-2061.	3.0	104
65	The importance of an accurate CH4 vibrational partition function in full dimensionality calculations of the H+CH4â†'H2+CH3 reaction. Journal of Chemical Physics, 2001, 114, 9683-9684.	3.0	89
66	Reactantâ€"product decoupling approach to state-to-state dynamics calculation for bimolecular reaction and unimolecular fragmentation. Faraday Discussions, 1998, 110, 159-167.	3.2	19
67	Correction of repulsive potential energy surface for photodissociation of H2O in the Ãƒ state. Journal of Chemical Physics, 1998, 108, 10027-10032.	3.0	3
68	Reactant-product decoupling approach to half-scattering problems: Photodissociation of H2O in three dimensions. Journal of Chemical Physics, 1997, 107, 751-756.	3.0	8
69	Quantum dynamics study of Li + HF reaction. Theoretical Chemistry Accounts, 1997, 96, 31-38.	1.4	44
70	Quantum calculation of photodetachment spectrum of OHâ^'(H2). Chemical Physics Letters, 1997, 273, 171-178.	2.6	11
71	Quantum dynamics study of the reaction HD+OHâ†'H+DOH, D+HOH. Journal of Chemical Physics, 1995, 102, 7400-7408.	3.0	72