Hyung J Kim

List of Publications by Year
in descending order

116 papers	5,949 citations	66343 42 h-index	76900 74 g-index
120 all docs	120 docs citations	120 times ranked	5610 citing authors

#	Article	IF	Citations
1	Mass spectrum of chiral ten-dimensionalN=2supergravity onS5. Physical Review D, 1985, 32, 389-399.	4.7	421
2	Gold Nanoclusters Promote Electrocatalytic Water Oxidation at the Nanocluster/CoSe₂ Interface. Journal of the American Chemical Society, 2017, 139, 1077-1080.	13.7	294
3	Nanoporous Carbon Supercapacitors in an Ionic Liquid: A Computer Simulation Study. ACS Nano, 2010, 4, 2345-2355.	14.6	267
4	Tailoring the Electronic and Catalytic Properties of Au₂₅ Nanoclusters via Ligand Engineering. ACS Nano, 2016, 10, 7998-8005.	14.6	175
5	Equilibrium and nonequilibrium solvation and solute electronic structure. III. Quantum theory. Journal of Chemical Physics, 1992, 96, 5088-5110.	3.0	166
6	Solvation in molecular ionic liquids. Journal of Chemical Physics, 2003, 119, 6411-6414.	3.0	156
7	Molecular Interactions of a Cu-Based Metalâ€“Organic Framework with a Confined Imidazolium-Based Ionic Liquid: A Combined Density Functional Theory and Experimental Vibrational Spectroscopy Study. Journal of Physical Chemistry C, 2016, 120, 3295-3304.	3.1	155
8	Equilibrium and nonequilibrium solvation and solute electronic structure. I. Formulation. Journal of Chemical Physics, 1990, 93, 5194-5210.	3.0	154
9	Silicon Nanoparticles with Surface Nitrogen: 90% Quantum Yield with Narrow Luminescence Bandwidth and the Ligand Structure Based Energy Law. ACS Nano, 2016, 10, 8385-8393.	14.6	154
10	Solvation of Carbon Nanotubes in a Room-Temperature Ionic Liquid. ACS Nano, 2009, 3, 1693-1702.	14.6	140
11	Chiral Ag23 nanocluster with open shell electronic structure and helical face-centered cubic framework. Nature Communications, 2018, 9, 744.	12.8	132
12	Revisiting the Aqueous Solutions of Dimethyl Sulfoxide by Spectroscopy in the Mid- and Near-Infrared: Experiments and Carâ€“Parrinello Simulations. Journal of Physical Chemistry B, 2015, 119, 14780-14789.	2.6	129
13	A theoretical model for SN1 ionic dissociation in solution. 1. Activation free energetics and transition-state structure. Journal of the American Chemical Society, 1992, 114, 10508-10528.	13.7	117
14	Free energies of electron transfer. The Journal of Physical Chemistry, 1992, 96, 1748-1753.	2.9	112
15	A molecular dynamics computer simulation study of room-temperature ionic liquids. II. Equilibrium and nonequilibrium solvation dynamics. Journal of Chemical Physics, 2005, 122, 044511.	3.0	105
16	Graphene-Based Supercapacitors: A Computer Simulation Study. Journal of Physical Chemistry C, 2011, 115, 23574-23583.	3.1	104
17	Molecular Interactions in 1-Ethyl-3-methylimidazolium Acetate Ion Pair: A Density Functional Study. Journal of Physical Chemistry A, 2009, 113, 10397-10404.	2.5	97
18	Experimental and Mechanistic Understanding of Aldehyde Hydrogenation Using Au₂₅ Nanoclusters with Lewis Acids: Unique Sites for Catalytic Reactions. Journal of the American Chemical Society, 2015, 137, 14295-14304.	13.7	95

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19	Molecular Dynamics Study of Water Flow across Multiple Layers of Pristine, Oxidized, and Mixed Regions of Graphene Oxide. ACS Nano, 2017, 11, 2187-2193.	14.6	92
20	Dielectric Relaxation, Ion Conductivity, Solvent Rotation, and Solvation Dynamics in a Room-Temperature Ionic Liquid. Journal of Physical Chemistry B, 2008, 112, 11028-11038.	2.6	91
21	Molecular Structure and Interactions in the Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(Trifluoromethylsulfonyl)imide. Journal of Physical Chemistry A, 2014, 118, 2547-2557.	2.5	90
22	A molecular dynamics computer simulation study of room-temperature ionic liquids. I. Equilibrium solvation structure and free energetics. Journal of Chemical Physics, 2005, 122, 044510.	3.0	84
23	Equilibrium and nonequilibrium solvation and solute electronic structure. II. Strong coupling limit. Journal of Chemical Physics, 1990, 93, 5211-5223.	3.0	79
24	Graphene-based supercapacitors in the parallel-plate electrode configuration: Ionic liquidsversus organic electrolytes. Faraday Discussions, 2012, 154, 249-263.	3.2	79
25	Solvation, Solute Rotation and Vibration Relaxation, and Electron-Transfer Reactions in Room-Temperature Ionic Liquids. Accounts of Chemical Research, 2007, 40, 1130-1137.	15.6	78
26	Shuttling single metal atom into and out of a metal nanoparticle. Nature Communications, 2017, 8, 848.	12.8	77
27	Electronic Structure and Normal Vibrations of the 1-Ethyl-3-methylimidazolium Ethyl Sulfate Ion Pair. Journal of Physical Chemistry A, 2011, 115, 3551-3558.	2.5	76
28	Role of solvent electronic polarization in electron-transfer processes. The Journal of Physical Chemistry, 1990, 94, 2736-2740.	2.9	67
29	Free Energy and Dynamics of Electron-Transfer Reactions in a Room Temperature Ionic Liquid. Journal of Physical Chemistry B, 2007, 111, 4510-4519.	2.6	64
30	Influence of Water on the Chemistry and Structure of the Metalâ€“Organic Framework Cu₃(btc)₂. Journal of Physical Chemistry C, 2016, 120, 17323-17333.	3.1	64
31	A theoretical model for SN1 ionic dissociation in solution. 2. Nonequilibrium solvation reaction path and reaction rate. Journal of the American Chemical Society, 1992, 114, 10528-10537.	13.7	61
32	Spectroscopic and dielectric properties of liquid water: A molecular dynamics simulation study. Journal of Chemical Physics, 1998, 109, 4911-4919.	3.0	60
33	Graphene Oxide Supercapacitors: A Computer Simulation Study. Journal of Physical Chemistry C, 2014, 118, 18472-18480.	3.1	60
34	Role of Solute Electronic Polarizability in Solvation Dynamics. The Journal of Physical Chemistry, 1995, 99, 10069-10074.	2.9	56
35	Effects of Solute Electronic Polarizability on Solvation in a Room-Temperature Ionic Liquidâ€. Journal of Physical Chemistry B, 2007, 111, 4920-4925.	2.6	53
36	A theoretical model for SN1 ionic dissociations in solution. 3. Analysis of tert-butyl halides. Journal of the American Chemical Society, 1993, 115, 8248-8262.	13.7	52

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37	Dynamics of twisted intramolecular charge transfer complexes in polar solvents. Journal of Molecular Liquids, 1994, 60, 161-200.	4.9	52
38	Excited state intramolecular charge transfer rates of p-dirnethylaminobenzonitrile (DMABN) in solution: a two-dimensional dynamics perspective. Journal of Photochemistry and Photobiology A: Chemistry, 1997, 105, 337-343.	3.9	51
39	Fragility, Stokesâ€“Einstein violation, and correlated local excitations in a coarse-grained model of an ionic liquid. Physical Chemistry Chemical Physics, 2010, 12, 2001.	2.8	48
40	Electronically adiabatic reaction field approach to solvation. I. Theoretical formulation via multipole expansion in a fluctuating cavity. Journal of Chemical Physics, 1996, 105, 6818-6832.	3.0	47
41	Molecular mechanism for the activation of Au25(SCH2CH2Ph)18 nanoclusters by imidazolium-based ionic liquids for catalysis. Journal of Catalysis, 2016, 337, 72-79.	6.2	47
42	On the Photoabsorption Spectroscopy of Water. Journal of Physical Chemistry A, 2000, 104, 45-52.	2.5	43
43	Generalized molecular mechanics including quantum electronic structure variation of polar solvents. II. A molecular dynamics simulation study of water. Journal of Chemical Physics, 1998, 108, 3286-3295.	3.0	42
44	Perfusion analysis using dynamic arterial spin labeling (DASL). Magnetic Resonance in Medicine, 1999, 41, 299-308.	3.0	42
45	A mechanistic insight into the organocatalytic properties of imidazolium-based ionic liquids and a positive co-solvent effect on cellulose modification reactions in an ionic liquid. RSC Advances, 2017, 7, 9423-9430.	3.6	41
46	Twisted intramolecular charge transfer dynamics in polar solvents. Journal of Photochemistry and Photobiology A: Chemistry, 1994, 82, 67-79.	3.9	39
47	Computer Simulation Study of Graphene Oxide Supercapacitors: Charge Screening Mechanism. Journal of Physical Chemistry Letters, 2016, 7, 1180-1186.	4.6	38
48	Understanding the mechanism of CO₂ capture by 1,3 di-substituted imidazolium acetate based ionic liquids. Physical Chemistry Chemical Physics, 2016, 18, 1911-1917.	2.8	37
49	Molecular Dynamics Simulation Study of Polarizable Solute Solvation in Water.Â 1. Equilibrium Solvent Structure and Solute Rotational Dynamics. The Journal of Physical Chemistry, 1996, 100, 1392-1405.	2.9	36
50	Rotational dynamics of a diatomic solute in the room-temperature ionic liquid 1-ethyl-3-methylimidazolium hexafluorophosphate. Journal of Chemical Physics, 2006, 125, 061102.	3.0	36
51	Influence of methyl and propyl groups on the vibrational spectra of two imidazolium ionic liquids and their non-ionic precursors. Journal of Molecular Structure, 2017, 1134, 582-590.	3.6	36
52	Inducing Coherent Oscillations in the Electron Transfer Dynamics of a Strongly Dissipative System with Pulsed Monochromatic Light. Physical Review Letters, 1995, 75, 3649-3652.	7.8	35
53	Smoluchowski fluctuation theory of dielectric relaxation. Journal of Chemical Physics, 1991, 94, 1442-1453.	3.0	34
54	A simple basis set approach to solute electronic structure and free energy in solution. The Journal of Physical Chemistry, 1993, 97, 1723-1728.	2.9	34

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55	Electronically adiabatic reaction field approach to solvation. II. Solvent effects on electronic spectra. Journal of Chemical Physics, 1996, 105, 6833-6843.	3.0	34
56	Molecular-like Transformation from PhSe-Protected Au₂₅ to Au₂₃ Nanocluster and Its Application. Chemistry of Materials, 2017, 29, 3055-3061.	6.7	34
57	Adiabatic Electron Transfer in a Room-Temperature Ionic Liquid: Reaction Dynamics and Kinetics. Journal of Physical Chemistry B, 2009, 113, 12964-12972.	2.6	32
58	Effect of Magnesium on Calcium and Oxalate Ion Binding. Journal of Endourology, 2013, 27, 1487-1492.	2.1	32
59	Excited-State Charge Transfer Dynamics ofp-Dimethylaminobenzonitrile in Quadrupolar Solventsâ€. Journal of Physical Chemistry A, 2002, 106, 2322-2327.	2.5	30
60	Dielectric Relaxation and Solvation Dynamics in a Room-Temperature Ionic Liquid: Temperature Dependence. Journal of Physical Chemistry B, 2013, 117, 11743-11752.	2.6	29
61	MD Study of Solvation in the Mixture of a Room-Temperature Ionic Liquid and CO₂. Journal of Physical Chemistry B, 2010, 114, 10160-10170.	2.6	28
62	CO₂ capture in ionic liquid 1-alkyl-3-methylimidazolium acetate: a concerted mechanism without carbene. Physical Chemistry Chemical Physics, 2017, 19, 1361-1368.	2.8	28
63	Goldâ€“Palladium Nanoalloys Supported by Graphene Oxide and Lamellar TiO₂ for Direct Synthesis of Hydrogen Peroxide. ACS Applied Materials & Interfaces, 2018, 10, 40599-40607.	8.0	28
64	Molecular dynamics simulation study of water near critical conditions. I. Structure and solvation free energetics. Journal of Chemical Physics, 1999, 110, 9646-9655.	3.0	27
65	Free Energies of Electron Transfer Reactions in Polarizable, Nondipolar, Quadrupolar Solvents. Journal of Physical Chemistry A, 2000, 104, 9812-9815.	2.5	27
66	Molecular Dynamics Study of Water Flow Across Multiple Layers of Pristine, Oxidized, and Mixed Regions of Graphene Oxide: Effect of Graphene Oxide Layer-to-Layer Distance. Journal of Physical Chemistry C, 2017, 121, 23659-23668.	3.1	26
67	Generalized molecular mechanics including quantum electronic structure variation of polar solvents. I. Theoretical formulation via a truncated adiabatic basis set description. Journal of Chemical Physics, 1998, 108, 3277-3285.	3.0	24
68	A molecular dynamics study of the ionic liquid, choline acetate. Physical Chemistry Chemical Physics, 2016, 18, 14850-14858.	2.8	24
69	A continuum theory of solvation in quadrupolar solvents. II. Solvation free energetics, dynamics, and solvatochromism. Journal of Chemical Physics, 2003, 119, 8626-8635.	3.0	23
70	Silica-Encapsulated Gold Nanoclusters for Efficient Acetylene Hydrogenation to Ethylene. ACS Applied Nano Materials, 2019, 2, 2999-3006.	5.0	23
71	Carbon nanotubes in benzene: internal and external solvation. Physical Chemistry Chemical Physics, 2011, 13, 3969.	2.8	22
72	Optical Kerr Effect Spectroscopy of Liquid Water:Â Role of Fluctuating Electronic Polarizability. Journal of Physical Chemistry B, 1997, 101, 10994-10999.	2.6	21

#	Article	IF	Citations
73	Title is missing!. Journal of Solution Chemistry, 2001, 30, 849-860.	1.2	21
74	Synthesis, conductivity, and vibrational spectroscopy of tetraphenylphosphonium bis(trifluoromethanesulfonyl)imide. Journal of Molecular Structure, 2017, 1146, 203-212.	3.6	21
75	Equilibrium and nonequilibrium solvation and solute electronic structure. International Journal of Quantum Chemistry, 1990, 38, 821-833.	2.0	20
76	The effect of a laser field on electron transfer in metal complexes: Quantum degrees of freedom. Journal of Chemical Physics, 1995, 103, 5461-5469.	3.0	20
77	Effects of Solute Electronic Structure Variation on Photon Echo Spectroscopy. The Journal of Physical Chemistry, 1996, 100, 16451-16456.	2.9	20
78	Molecular dynamics simulation study of water near critical conditions. II. Dynamics and spectroscopy. Journal of Chemical Physics, 1999, 110, 9656-9665.	3.0	20
79	A continuum theory of solvation in quadrupolar solvents. I. Formulation. Journal of Chemical Physics, 2003, 119, 8606-8625.	3.0	20
80	Solvation in supercritical water. Journal of Chemical Physics, 2006, 124, 204504.	3.0	20
81	Dielectric relaxation of hot water. Journal of Chemical Physics, 2000, 113, 6025-6028.	3.0	18
82	1 âˆ• f spectrum and memory function analysis of solvation dynamics in a room-temperature ionic liquid. Journal of Chemical Physics, 2008, 128, 174504.	3.0	18
83	Spectroscopic and MD Study of Dynamic and Structural Heterogeneities in Ionic Liquids. Journal of Physical Chemistry B, 2017, 121, 1100-1107.	2.6	18
84	Solute electronic structure and solvation in chemical reactions in solution. Journal of Molecular Liquids, 1993, 57, 53-73.	4.9	16
85	On the structural stability of ionic liquidâ€“IRMOF composites: a computational study. Physical Chemistry Chemical Physics, 2015, 17, 6248-6254.	2.8	16
86	Vibrational energy relaxation of a diatomic molecule in a room-temperature ionic liquid. Journal of Chemical Physics, 2006, 125, 024507.	3.0	15
87	Electrostriction effects on electron transfer reactions in solution. I. Adiabatic regime. Journal of Chemical Physics, 1997, 106, 5979-5989.	3.0	14
88	Conformational Dynamics and Ligand Binding in the Multi-Domain Protein PDC109. PLoS ONE, 2010, 5, e9180.	2.5	14
89	Theoretical study of interactions of a Li⁺(CF₃SO₂)₂N^{â^'} ion pair with CR₃(OCR₂CR₂)_nOCR₃ (R = H or F). Physical Chemistry Chemical Physics, 2016, 18, 6754-6762.	2.8	14
90	Dielectric Relaxation of the Ionic Liquid 1-Ethyl-3-methylimidazolium Ethyl Sulfate: Microwave and Far-IR Properties. Journal of Physical Chemistry B, 2017, 121, 4845-4852.	2.6	14

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91	MD Study of Stokes Shifts in Ionic Liquids: Temperature Dependence. Journal of Physical Chemistry B, 2016, 120, 4644-4653.	2.6	13
92	Removal of Confined Ionic Liquid from a Metal Organic Framework by Extraction with Molecular Solvents. Journal of Physical Chemistry C, 2017, 121, 10577-10586.	3.1	12
93	Temperature- and Pressure-Dependence of the Outer-Sphere Reorganization Free Energy for Electron Transfer Reactions:Â A Continuum Approach. Journal of Physical Chemistry B, 2006, 110, 494-500.	2.6	11
94	MD Study of S_N1 Reactivity of 2-Chloro-2-methylpropane in the Room-Temperature Ionic Liquid 1-Ethyl-3-methylimidazolium Hexafluorophosphate. Journal of Physical Chemistry B, 2008, 112, 2637-2643.	2.6	11
95	Heterogeneous dynamics of ionic liquids: A four-point time correlation function approach. Journal of Chemical Physics, 2018, 148, 193830.	3.0	11
96	On the temperature and pressure dependences of cavities in the dielectric continuum picture. Journal of Chemical Physics, 2005, 123, 014504.	3.0	10
97	CS2 capture in the ionic liquid 1-alkyl-3-methylimidazolium acetate: reaction mechanism and free energetics. Physical Chemistry Chemical Physics, 2018, 20, 19339-19349.	2.8	7
98	Computer-Aided Design of Postpolymerization Modification Reaction Based on Aminolysis of Î±,Î±-Difluoroacetate Esters. Macromolecules, 2021, 54, 364-372.	4.8	7
99	Smoluchowski fluctuation theory of ion transport in solutions. Journal of Chemical Physics, 1988, 89, 3222-3232.	3.0	6
100	Quantum tunneling in an anharmonic classical bath. Enhanced kinetic isotope effects in an Arrhenius region. Journal of Chemical Physics, 1995, 102, 7838-7849.	3.0	6
101	Excitation-energy dependence of solvation dynamics in room-temperature ionic liquids. Journal of Chemical Physics, 2016, 145, 044502.	3.0	6
102	Vibrational spectroscopy of imidazolium-based ionic liquids: A combined MD/DFT study. Journal of Molecular Liquids, 2019, 292, 111282.	4.9	6
103	Solvation of a Small Metal-Binding Peptide in Room-Temperature Ionic Liquids. Bulletin of the Korean Chemical Society, 2012, 33, 3601-3606.	1.9	6
104	Solvent Dynamics and Charge Transfer Reactions. , 1992, , 39-56.		5
105	Electron-Transfer Reactions in Supercritical Water. Journal of Physical Chemistry B, 2008, 112, 585-594.	2.6	4
106	Dicationic-Type Quaternary Ammonium Salts as Candidates of Desiccants for an Air-Conditioning System. ACS Sustainable Chemistry and Engineering, 2021, 9, 14502-14514.	6.7	4
107	Fundamental insights into aminolysis postpolymerization modification reaction of polymers featuring Î±,Î±-Difluoroacetate Esters. Polymer, 2021, 230, 124058.	3.8	3
108	Mass Spectrometry of Au₁₀(4-tert-butylbenzenethiolate)₁₀ Nanoclusters Using Superconducting Tunnel Junction Cryodetection Reveals Distinct Metastable Fragmentation. Journal of the American Society for Mass Spectrometry, 2022, 33, 521-529.	2.8	3

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109	Solubility of Water in a Benzeneâ^'Cyclohexane Mixtureâ€. Journal of Physical Chemistry A, 2006, 110, 429-435.	2.5	2
110	Free energy, entropy and volume of activation for electron transfer reactions in a polar solvent. Journal of Chemical Physics, 2006, 125, 011101.	3.0	2
111	<title>Computer simulation study of electronic spectroscopy in water</title>. , 1998, , .		1
112	Theoretical Study of Alkylsulfonic Acids: Force-Field Development and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2018, 122, 9747-9756.	2.6	1
113	Deconvolution of conformational equilibria in methimazolium-based ionic liquid ion pair: Infrared spectroscopic and computational study. Journal of Molecular Liquids, 2018, 266, 194-202.	4.9	1
114	Perfusion analysis using dynamic arterial spin labeling (DASL). Magnetic Resonance in Medicine, 1999, 41, 299-308.	3.0	1
115	Generalized Molecular Mechanics Including Quantum Electronic Structure Variation of Polar Solvents: An Overview. ACS Symposium Series, 1998, , 172-187.	0.5	0
116	Electronic Structure and Chemical Reactions in Solution. Jerusalem Symposia on Quantum Chemistry and Biochemistry, 1994, , 289-309.	0.2	0