Edward Kober

List of Publications by Year
in descending order

68 papers	5,487 citations	117625 34 h-index	102487 66 g-index
84 all docs	84 docs citations	84 times ranked	4448 citing authors

#	Article	IF	Citations
1	Application of the energy gap law to the decay of charge-transfer excited states. Journal of the American Chemical Society, 1982, 104, 630-632.	13.7	605
2	Application of the energy gap law to excited-state decay of osmium(II)-polypyridine complexes: calculation of relative nonradiative decay rates from emission spectral profiles. The Journal of Physical Chemistry, 1986, 90, 3722-3734.	2.9	578
3	Simulations on the Thermal Decomposition of a Poly(dimethylsiloxane) Polymer Using the ReaxFF Reactive Force Field. Journal of the American Chemical Society, 2005, 127, 7192-7202.	13.7	395
4	Thermal decomposition of RDX from reactive molecular dynamics. Journal of Chemical Physics, 2005, 122, 054502.	3.0	366
5	Synthetic routes to new polypyridyl complexes of osmium(II). Inorganic Chemistry, 1988, 27, 4587-4598.	4.0	339
6	Concerning the absorption spectra of the ions M(bpy)32+ (M = Fe, Ru, Os; bpy = 2,2'-bipyridine). Inorganic Chemistry, 1982, 21, 3967-3977.	4.0	320
7	Carbon Cluster Formation during Thermal Decomposition of Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine and 1,3,5-Triamino-2,4,6-trinitrobenzene High Explosives from ReaxFF Reactive Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2009, 113, 10619-10640.	2.5	257
8	Solvent dependence of metal-to-ligand charge-transfer transitions. Evidence for initial electron localization in MLCT excited states of 2,2'-bipyridine complexes of ruthenium(II) and osmium(II). Inorganic Chemistry, 1984, 23, 2098-2104.	4.0	201
9	Metal-to-ligand charge-transfer (MLCT) photochemistry: experimental evidence for the participation of a higher lying MLCT state in polypyridyl complexes of ruthenium(II) and osmium(II). The Journal of Physical Chemistry, 1990, 94, 239-243.	2.9	192
10	Synthetic control of excited states. Nonchromophoric ligand variations in polypyridyl complexes of osmium(II). Inorganic Chemistry, 1985, 24, 2755-2763.	4.0	171
11	Influence of Solvent on the Spectroscopic Properties of Cyano Complexes of Ruthenium(II). The Journal of Physical Chemistry, 1996, 100, 2915-2925.	2.9	147
12	Highly luminescent polypyridyl complexes of osmium(II). Journal of the American Chemical Society, 1980, 102, 7383-7385.	13.7	140
13	An electronic structural model for the emitting MLCT excited states of Ru(bpy)32+ and Os(bpy)32+. Inorganic Chemistry, 1984, 23, 3877-3886.	4.0	140
14	Application of the energy gap law to the decay of charge transfer excited states, solvent effects. Chemical Physics Letters, 1982, 91, 91-95.	2.6	111
15	Ultrafast Chemistry under Nonequilibrium Conditions and the Shock to Deflagration Transition at the Nanoscale. Journal of Physical Chemistry C, 2015, 119, 22008-22015.	3.1	110
16	Electronic structure in the intervalence transfer absorption band of a mixed-valence dimer. Journal of the American Chemical Society, 1983, 105, 4303-4309.	13.7	75
17	Electronic coupling in mixed-valence binuclear ruthenium ammine complexes as probed by an electrochemical method and an extension of Mulliken's theory of donor-acceptor interactions. Inorganic Chemistry, 1993, 32, 3895-3908.	4.0	73
18	Concerning the electronic structure of the ions M(bpy)33+ (M = Fe, Ru, Os; bpy = 2,2'-bipyridine). Inorganic Chemistry, 1983, 22, 1614-1616.	4.0	71

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19	Cleavage of the triple bond in phenylacetylene by monomeric ruthenium(II) and osmium(II) complexes. Formation of stable ruthenium(II) alkyls from terminal alkynes. Journal of the American Chemical Society, 1982, 104, 4701-4703.	13.7	60
20	Intervalence Transfer at the Localized-to-Delocalized, Mixed-Valence Transition in Osmium Polypyridyl Complexes. Inorganic Chemistry, 1999, 38, 5948-5959.	4.0	60
21	Energy relationships in optical and thermal electron transfer. Temperature dependence of an intervalence transfer absorption band. The Journal of Physical Chemistry, 1992, 96, 10820-10830.	2.9	58
22	Electric Double-Layer Structure in Primitive Model Electrolytes: Comparing Molecular Dynamics with Local-Density Approximations. Langmuir, 2015, 31, 3553-3562.	3.5	55
23	A molecular dynamics simulation and quantum chemistry study of poly(dimethylsiloxane)â€“silica nanoparticle interactions. Journal of Polymer Science, Part B: Polymer Physics, 2007, 45, 1599-1615.	2.1	53
24	Examining the chemical and structural properties that influence the sensitivity of energetic nitrate esters. Chemical Science, 2018, 9, 3649-3663.	7.4	52
25	Shock Loading of Granular Ni/Al Composites. Part 1: Mechanics of Loading. Journal of Physical Chemistry C, 2014, 118, 26377-26386.	3.1	47
26	Vibrational Mapping at the Mixed-Valence, Localized-to-Delocalized Transition. Journal of the American Chemical Society, 1998, 120, 7121-7122.	13.7	45
27	Reactions of metal-metal multiple bonds. 14. Synthesis and characterization of triangulo-W3 and -Mo2W oxo-capped alkoxide clusters. Conproportionation of M-M triple bonds and .sigma.2.pi.4 and d0 metal-oxo groups: M.tplbond.M + M.tplbond.O .fwdarw. M3(.mu.3-O). Inorganic Chemistry, 1985, 24, 241-245.	4.0	43
28	Effects of hydrolysis-induced molecular weight changes on the phase separation of a polyester polyurethane. Polymer Degradation and Stability, 2006, 91, 3360-3370.	5.8	42
29	Unsupervised Learning-Based Multiscale Model of Thermochemistry in 1,3,5-Trinitro-1,3,5-triazinane (RDX). Journal of Physical Chemistry A, 2020, 124, 9141-9155.	2.5	41
30	Critical deactivating modes for the metal-2,2'-bipyridine or -1,10-phenanthroline MLCT excited states. Inorganic Chemistry, 1985, 24, 106-108.	4.0	39
31	Valence .sigma. ionization in systems with multiple metal-metal bonds. Journal of the American Chemical Society, 1985, 107, 7199-7201.	13.7	39
32	A molecular dynamics simulation study of the pressure-volume-temperature behavior of polymers under high pressure. Journal of Chemical Physics, 2009, 130, 144904.	3.0	39
33	The tungsten-tungsten triple bond. 13. Bisalkyl tetracarboxylates of dimolybdenum and ditungsten. Triple bonds between metal atoms with the valence molecular orbital description .pi.4.delta.2. Journal of the American Chemical Society, 1987, 109, 6796-6816.	13.7	37
34	Shock Loading of Granular Ni/Al Composites. Part 2: Shock-Induced Chemistry. Journal of Physical Chemistry C, 2016, 120, 6804-6813.	3.1	35
35	Characterization of bis(2,2'-bipyridine) and bis(1,10-phenanthroline) derivatives of molybdenum and tungsten carbonyls. Crystal and molecular structure of cis-dicarbonylbis(2,2'-bipyridine)molybdenum(0). Inorganic Chemistry, 1984, 23, 2298-2303.	4.0	34
36	A novel method for static equation-of state-development: Equation of state of a cross-linked poly(dimethylsiloxane) (PDMS) network to 10 GPa. Journal of Chemical Physics, 2005, 122, 144903.	3.0	31

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37	Mid-Infrared Spectrum of [Ru(phen)3]2+*. Inorganic Chemistry, 1998, 37, 3505-3508.	4.0	26
38	Morphology and bridging properties of (AB)n multiblock copolymers. Journal of Polymer Science, Part B: Polymer Physics, 2003, 41, 104-111.	2.1	26
39	Theoretical and experimental studies of the electronic structure of the Mo3(.mu.3-O)(.mu.3-OR)(.mu.-OR)3(OR)6 type of triangular metal atom cluster compound. Inorganic Chemistry, 1984, 23, 749-754.	4.0	24
40	95Mo and 183W NMR studies of triply bonded dinuclear M(III) and related Mî—¼C (M = Mo or W) complexes. Polyhedron, 1987, 6, 255-259.	2.2	23
41	Stress Distributions in Diblock Copolymers. Physical Review Letters, 2007, 99, 048302.	7.8	23
42	Vibrational and structural mapping of [Os(bpy)3]3+/2+ and [Os(phen)3]3+/2+. Inorganica Chimica Acta, 2007, 360, 1143-1153.	2.4	23
43	Calculation of grain boundary normals directly from 3D microstructure images. Modelling and Simulation in Materials Science and Engineering, 2015, 23, 035005.	2.0	20
44	Electron distribution and bonding in .eta.3-cyclopropenyl-metal complexes. Organometallics, 1993, 12, 2025-2031.	2.3	19
45	Probing ultrafast shock-induced chemistry in liquids using broad-band mid-infrared absorption spectroscopy. Journal of Chemical Physics, 2019, 150, 204503.	3.0	17
46	Molecular dynamics simulations of detonation instability. Physical Review E, 2008, 78, 046710.	2.1	16
47	Bis(2,2â€²-bipyridyl)diisopropoxomolybdenum(II): A spin-state equilibrium for a complex of a second-row transition element. Polyhedron, 1985, 4, 1869-1874.	2.2	15
48	1,3-Ditungstacyclobutadienes. 2. Synthesis of alkoxide derivatives of W2(.mu.-CSiMe3)2(CH2SiMe3)4 and investigations of the electronic structures of the M2(.mu.-CSiMe3)2 core as a function of dn-dn interactions (n = 0, M = Ta; n = 1, M = W; n = 2, M = Re). Organometallics, 1987, 6, 1065-1073.	2.3	15
49	Shape selection in the association of diaminoguanidinium cation with counterions. Journal of Organic Chemistry, 1990, 55, 1994-2000.	3.2	15
50	Application of time-resolved near-infrared spectroscopy (TRNIR) to the metal-to-ligand charge transfer (MLCT) excited state(s) of. Chemical Physics, 2006, 326, 71-78.	1.9	15
51	Phase segregation of diblock copolymers in nanopore geometries. Europhysics Letters, 2008, 81, 56001.	2.0	14
52	Parallel replica dynamics simulations of reactions in shock compressed liquid benzene. Journal of Chemical Physics, 2019, 150, 244108.	3.0	13
53	Thermodynamic and Conformational Changes upon Stretching a Poly(dimethylsiloxane) Chain in the Melt. Macromolecules, 2005, 38, 8101-8107.	4.8	12
54	Influence of interatomic bonding potentials on detonation properties. Physical Review E, 2007, 76, 026318.	2.1	12

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55	Vibrational Analysis of the Inelastic Neutron Scattering Spectrum of Tetramethylammonium Borohydride by Molecular Dynamics Simulations and Electronic Structure Calculations. Journal of Physical Chemistry A, 2004, 108, 11369-11374.	2.5	11
56	Interaction potential for atomic simulations of conventional high explosives. Physical Review E, 2008, 78, 046709.	2.1	10
57	Model-free test of local-density mean-field behavior in electric double layers. Physical Review E, 2013, 88, 011301.	2.1	10
58	Electronic absorption spectra of M2L6 compounds containing metal-metal triple bonds of Ïƒ2Ï€4 configuration. Polyhedron, 1987, 6, 723-727.	2.2	9
59	Developing Reaction Chemistry Models from Reactive Molecular Dynamics: TATB. Propellants, Explosives, Pyrotechnics, 2022, 47, .	1.6	4
60	Monomeric alkene and alkyne complexes of osmium(II) and osmium(III). Organometallics, 1982, 1, 1011-1013.	2.3	2
61	MOLECULAR DYNAMICS STUDIES OF THERMAL INDUCED CHEMISTRY IN TATB. AIP Conference Proceedings, 2008, , .	0.4	2
62	Ordering and Reverse Ordering Mechanisms of Triblock Copolymers in the Presence of Solvent. International Journal of Molecular Sciences, 2009, 10, 805-816.	4.1	2
63	Morphology of diblock copolymers in porous media. Molecular Physics, 2014, 112, 2297-2309.	1.7	2
64	Effective particle size from molecular dynamics simulations in fluids. Theoretical and Computational Fluid Dynamics, 2018, 32, 215-233.	2.2	2
65	Solvent and Temperature Effects in Mixed-Valence Chemistry. , 1991, , 51-66.		2
66	A quantum chemical method for calculating vibrational line shifts in diatomic fluids. Chemical Physics Letters, 2008, 464, 265-270.	2.6	1
67	Accelerated Molecular Dynamics Simulations of Shock-Induced Chemistry: Application to Liquid Benzene. Challenges and Advances in Computational Chemistry and Physics, 2019, , 53-70.	0.6	1
68	Bridging Properties of Multiblock Copolymers. Materials Research Society Symposia Proceedings, 2002, 734, 431.	0.1	0