Edward Kober

List of Publications by Year
in descending order

68 papers	5,487 citations	134610 34 h-index	116156 66 g-index
84 all docs	84 docs citations	84 times ranked	5019 citing authors

#	Article	IF	Citations
1	Developing Reaction Chemistry Models from Reactive Molecular Dynamics: TATB. Propellants, Explosives, Pyrotechnics, 2022, 47, .	1.0	4
2	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.	1.1	41
3	Parallel replica dynamics simulations of reactions in shock compressed liquid benzene. Journal of Chemical Physics, 2019, 150, 244108.	1.2	13
4	Probing ultrafast shock-induced chemistry in liquids using broad-band mid-infrared absorption spectroscopy. Journal of Chemical Physics, 2019, 150, 204503.	1.2	17
5	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
6	Examining the chemical and structural properties that influence the sensitivity of energetic nitrate esters. Chemical Science, 2018, 9, 3649-3663.	3.7	52
7	Effective particle size from molecular dynamics simulations in fluids. Theoretical and Computational Fluid Dynamics, 2018, 32, 215-233.	0.9	2
8	Shock Loading of Granular Ni/Al Composites. Part 2: Shock-Induced Chemistry. Journal of Physical Chemistry C, 2016, 120, 6804-6813.	1.5	35
9	Ultrafast Chemistry under Nonequilibrium Conditions and the Shock to Deflagration Transition at the Nanoscale. Journal of Physical Chemistry C, 2015, 119, 22008-22015.	1.5	110
10	Calculation of grain boundary normals directly from 3D microstructure images. Modelling and Simulation in Materials Science and Engineering, 2015, 23, 035005.	0.8	20
11	Electric Double-Layer Structure in Primitive Model Electrolytes: Comparing Molecular Dynamics with Local-Density Approximations. Langmuir, 2015, 31, 3553-3562.	1.6	55
12	Morphology of diblock copolymers in porous media. Molecular Physics, 2014, 112, 2297-2309.	0.8	2
13	Shock Loading of Granular Ni/Al Composites. Part 1: Mechanics of Loading. Journal of Physical Chemistry C, 2014, 118, 26377-26386.	1.5	47
14	Model-free test of local-density mean-field behavior in electric double layers. Physical Review E, 2013, 88, 011301.	0.8	10
15	A molecular dynamics simulation study of the pressure-volume-temperature behavior of polymers under high pressure. Journal of Chemical Physics, 2009, 130, 144904.	1.2	39
16	Ordering and Reverse Ordering Mechanisms of Triblock Copolymers in the Presence of Solvent. International Journal of Molecular Sciences, 2009, 10, 805-816.	1.8	2
17	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.	1.1	257
18	A quantum chemical method for calculating vibrational line shifts in diatomic fluids. Chemical Physics Letters, 2008, 464, 265-270.	1.2	1

#	Article	IF	Citations
19	Phase segregation of diblock copolymers in nanopore geometries. Europhysics Letters, 2008, 81, 56001.	0.7	14
20	Molecular dynamics simulations of detonation instability. Physical Review E, 2008, 78, 046710.	0.8	16
21	Interaction potential for atomic simulations of conventional high explosives. Physical Review E, 2008, 78, 046709.	0.8	10
22	MOLECULAR DYNAMICS STUDIES OF THERMAL INDUCED CHEMISTRY IN TATB. AIP Conference Proceedings, 2008, , .	0.3	2
23	Influence of interatomic bonding potentials on detonation properties. Physical Review E, 2007, 76, 026318.	0.8	12
24	Stress Distributions in Diblock Copolymers. Physical Review Letters, 2007, 99, 048302.	2.9	23
25	Vibrational and structural mapping of [Os(bpy)3]3+/2+ and [Os(phen)3]3+/2+. Inorganica Chimica Acta, 2007, 360, 1143-1153.	1.2	23
26	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.	2.4	53
27	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.	0.9	15
28	Effects of hydrolysis-induced molecular weight changes on the phase separation of a polyester polyurethane. Polymer Degradation and Stability, 2006, 91, 3360-3370.	2.7	42
29	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.	1.2	31
30	Thermodynamic and Conformational Changes upon Stretching a Poly(dimethylsiloxane) Chain in the Melt. Macromolecules, 2005, 38, 8101-8107.	2.2	12
31	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.	6.6	395
32	Thermal decomposition of RDX from reactive molecular dynamics. Journal of Chemical Physics, 2005, 122, 054502.	1.2	366
33	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.	1.1	11
34	Morphology and bridging properties of (AB)n multiblock copolymers. Journal of Polymer Science, Part B: Polymer Physics, 2003, 41, 104-111.	2.4	26
35	Bridging Properties of Multiblock Copolymers. Materials Research Society Symposia Proceedings, 2002, 734, 431.	0.1	0
36	Intervalence Transfer at the Localized-to-Delocalized, Mixed-Valence Transition in Osmium Polypyridyl Complexes. Inorganic Chemistry, 1999, 38, 5948-5959.	1.9	60

#	Article	IF	Citations
37	Vibrational Mapping at the Mixed-Valence, Localized-to-Delocalized Transition. Journal of the American Chemical Society, 1998, 120, 7121-7122.	6.6	45
38	Mid-Infrared Spectrum of [Ru(phen)3]2+*. Inorganic Chemistry, 1998, 37, 3505-3508.	1.9	26
39	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
40	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.	1.9	73
41	Electron distribution and bonding in .eta.3-cyclopropenyl-metal complexes. Organometallics, 1993, 12, 2025-2031.	1.1	19
42	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
43	Solvent and Temperature Effects in Mixed-Valence Chemistry. , 1991, , 51-66.		2
44	Shape selection in the association of diaminoguanidinium cation with counterions. Journal of Organic Chemistry, 1990, 55, 1994-2000.	1.7	15
45	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
46	Synthetic routes to new polypyridyl complexes of osmium(II). Inorganic Chemistry, 1988, 27, 4587-4598.	1.9	339
47	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.	1.1	15
48	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.	6.6	37
49	Electronic absorption spectra of M2L6 compounds containing metal-metal triple bonds of Ïƒ2Ï€4 configuration. Polyhedron, 1987, 6, 723-727.	1.0	9
50	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.	1.0	23
51	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
52	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.	1.0	15
53	Synthetic control of excited states. Nonchromophoric ligand variations in polypyridyl complexes of osmium(II). Inorganic Chemistry, 1985, 24, 2755-2763.	1.9	171
54	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.	1.9	43

#	Article	IF	Citations
55	Critical deactivating modes for the metal-2,2'-bipyridine or -1,10-phenanthroline MLCT excited states. Inorganic Chemistry, 1985, 24, 106-108.	1.9	39
56	Valence .sigma. ionization in systems with multiple metal-metal bonds. Journal of the American Chemical Society, 1985, 107, 7199-7201.	6.6	39
57	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.	1.9	24
58	An electronic structural model for the emitting MLCT excited states of Ru(bpy)32+ and Os(bpy)32+. Inorganic Chemistry, 1984, 23, 3877-3886.	1.9	140
59	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.	1.9	34
60	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.	1.9	201
61	Concerning the electronic structure of the ions M(bpy)33+ (M = Fe, Ru, Os; bpy = 2,2'-bipyridine). Inorganic Chemistry, 1983, 22, 1614-1616.	1.9	71
62	Electronic structure in the intervalence transfer absorption band of a mixed-valence dimer. Journal of the American Chemical Society, 1983, 105, 4303-4309.	6.6	75
63	Concerning the absorption spectra of the ions M(bpy)32+ (M = Fe, Ru, Os; bpy = 2,2'-bipyridine). Inorganic Chemistry, 1982, 21, 3967-3977.	1.9	320
64	Monomeric alkene and alkyne complexes of osmium(II) and osmium(III). Organometallics, 1982, 1, 1011-1013.	1.1	2
65	Application of the energy gap law to the decay of charge-transfer excited states. Journal of the American Chemical Society, 1982, 104, 630-632.	6.6	605
66	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.	6.6	60
67	Application of the energy gap law to the decay of charge transfer excited states, solvent effects. Chemical Physics Letters, 1982, 91, 91-95.	1.2	111
68	Highly luminescent polypyridyl complexes of osmium(II). Journal of the American Chemical Society, 1980, 102, 7383-7385.	6.6	140