Koblar Alan Jackson

List of Publications by Citations

103 papers	22,812 citations	34 h-index	108 g-index
108 ext. papers	24,121 ext. citations	3.6 avg, IF	6.06 L-index

#	Paper	IF	Citations
103	Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation. *Physical Review B*, **1992**, 46, 6671-6687	3.3	17224
102	Variational mesh for quantum-mechanical simulations. *Physical Review B*, **1990**, 41, 7453-7461	3.3	438
101	Accurate forces in a local-orbital approach to the local-density approximation. *Physical Review B*, **1990**, 42, 3276-3281	3.3	325
100	Single-parent evolution algorithm and the optimization of Si clusters. *Physical Review Letters*, **2000**, 85, 546-9	7.4	179
99	Shape of small silicon clusters. *Physical Review Letters*, **1993**, 71, 727-730	7.4	163
98	Raman-active modes of α-GeSe2 and α-GeS2: A first-principles study. *Physical Review B*, **1999**, 60, R14985-R14989	3.3	156
97	Unraveling the Shape Transformation in Silicon Clusters. *Physical Review Letters*, **2004**, 93,	7.4	141
96	Pseudoenergies for simulations on metallic systems. *Physical Review B*, **1991**, 43, 7312-7315	3.3	136
95	Theory of magnetic and structural ordering in iron clusters. *Physical Review B*, **1991**, 44, 6558-6561	3.3	99
94	Zr@Si20: a strongly bound Si endohedral system. *Chemical Physics Letters*, **1996**, 254, 249-256	2.5	95
93	Structure and shape variations in intermediate-size copper clusters. *Journal of Chemical Physics*, **2006**, 124, 024308	3.9	93
92	Structure and vibrational spectra of low-energy silicon clusters. *Physical Review A*, **1997**, 56, 4890-4898	2.6	84
91	First-principles study of the structural and electronic properties of Cu clusters. *Physical Review B*, **1993**, 47, 9715-9722	3.3	79
90	Vibrational frequencies and intensities of small molecules: All-electron, pseudopotential, and mixed-potential methodologies. *Physical Review B*, **1998**, 58, 1786-1793	3.3	68
89	Density-functional-based predictions of Raman and IR spectra for small Si clusters. *Physical Review B*, **1997**, 55, 2549-2555	3.3	67
88	Calculated polarizabilities of intermediate-size Si clusters. *Physical Review A*, **1999**, 59, 3685-3689	2.6	67
87	Scanning the potential energy surface of iron clusters: A novel search strategy. *Journal of Chemical Physics*, **2002**, 116, 3576-3587	3.9	66

86	Optical absorption spectra of intermediate-size silver clusters from first principles. *Physical Review B*, **2008**, 78,	3.3	64
85	First-principles study of intermediate size silver clusters: Shape evolution and its impact on cluster properties. *Journal of Chemical Physics*, **2006**, 125, 144308	3.9	64
84	Sharp Rigid to Floppy Phase Transition Induced by Dangling Ends in a Network Glass. *Physical Review Letters*, **2001**, 87,	7.4	58
83	Local-density-approximation-based simulations of hydrocarbon interactions with applications to diamond chemical vapor deposition. *Physical Review B*, **1991**, 44, 3891-3899	3.3	57
82	Bonding of Endohedral Atoms in Small Carbon Fullerenes. *The Journal of Physical Chemistry*, **1994**, 98, 7805-7810		48
81	Donor levels and impurity-atom relaxation in nitrogen- and phosphorus-doped diamond. *Physical Review B*, **1990**, 41, 12641-12649	3.3	46
80	Shape transition of medium-sized neutral silicon clusters. *Physica Status Solidi (B): Basic Research*, **2003**, 240, 537-548	1.3	43
79	First-principles absorption spectra of Cun (n=2–20) clusters. *Physical Review B*, **2011**, 83,	3.3	39
78	The self-organized phase of bulk P x Se 1 − x glasses. *Europhysics Letters*, **2003**, 62, 49-55	1.6	39
77	Site-Specific Analysis of Dielectric Properties of Finite Systems. *Journal of Physical Chemistry C*, **2007**, 111, 17952-17960	3.8	38
76	Self-interaction error overbinds water clusters but cancels in structural energy differences. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 11283-11288	11.5	37
75	Hydrogenated and deuterated iron clusters: Infrared spectra and density functional calculations. *Journal of Chemical Physics*, **1998**, 109, 10692-10700	3.9	37
74	Vibrational signatures for low-energy intermediate-sized Si clusters. *Physical Review B*, **1996**, 54, 2863-2867	3.9	37
73	Electronic states of group-IV endohedral atoms in C28. *Physical Review B*, **1993**, 48, 17556-17561	3.3	36
72	Assessing student written problem solutions: A problem-solving rubric with application to introductory physics. *Physical Review Physics Education Research*, **2016**, 12,	2.3	36
71	Ball-and-Chain Dimers from a Hot Fullerene Plasma. *Journal of Physical Chemistry A*, **1999**, 103, 5275-5284	2.8	35
70	Self-consistent self-interaction corrected density functional theory calculations for atoms using Fermi-Löwdin orbitals: Optimized Fermi-orbital descriptors for Li-Kr. *Journal of Chemical Physics*, **2017**, 147, 164107	3.9	34
69	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. *Journal of Chemical Physics*, **2019**, 151, 214108	3.9	34

68	Stretched or noded orbital densities and self-interaction correction in density functional theory. *Journal of Chemical Physics*, **2019**, 150, 174102	3.9	33
67	Structure and energetics of SinNm clusters: Growth pathways in a heterogenous cluster system. *Journal of Chemical Physics*, **2000**, 112, 1295-1305	3.9	32
66	H2 reactions on palladium clusters. *Journal of Physical Chemistry A*, **2013**, 117, 10407-15	2.8	31
65	Icosahedral to double-icosahedral shape transition of copper clusters. *Journal of Chemical Physics*, **2012**, 136, 104501	3.9	31
64	First-principles investigations of the polarizability of small-sized and intermediate-sized copper clusters. *Journal of Chemical Physics*, **2005**, 122, 184317	3.9	30
63	New theoretical model for the diamond 1s core exciton. *Physical Review Letters*, **1991**, 67, 2521-2524	7.4	30
62	Fermi-L□wdin orbital self-interaction correction to magnetic exchange couplings. *Journal of Chemical Physics*, **2018**, 149, 164101	3.9	29
61	Structural growth behavior and polarizability of Cd(n)Te(n) (n=1-14) clusters. *Journal of Chemical Physics*, **2009**, 130, 214307	3.9	28
60	Theoretical investigation of adsorption of molecular oxygen on small copper clusters. *Journal of Physical Chemistry A*, **2011**, 115, 8705-12	2.8	27
59	Fermi-L□wdin orbital self-interaction correction using the strongly constrained and appropriately normed meta-GGA functional. *Journal of Chemical Physics*, **2019**, 151, 154105	3.9	27
58	Self-interaction-free electric dipole polarizabilities for atoms and their ions using the Fermi-L□wdin self-interaction correction. *Physical Review A*, **2019**, 100,	2.6	25
57	Shrinking Self-Interaction Errors with the Fermi-L□wdin Orbital Self-Interaction-Corrected Density Functional Approximation. *Journal of Physical Chemistry A*, **2018**, 122, 9307-9315	2.8	25
56	Importance of self-interaction-error removal in density functional calculations on water cluster anions. *Physical Chemistry Chemical Physics*, **2020**, 22, 3789-3799	3.6	24
55	The effect of self-interaction error on electrostatic dipoles calculated using density functional theory. *Journal of Chemical Physics*, **2019**, 151, 174106	3.9	23
54	Cage-forming tendencies in SinNm clusters. *Chemical Physics Letters*, **1998**, 292, 235-242	2.5	21
53	First-principles absorption spectra of Sin (n=20□8) clusters: Time-dependent local-density approximation versus predictions from Mie theory. *Physical Review B*, **2006**, 74,	3.3	21
52	Theoretical study of passivated small fullerenes C24X4 (X?N, P, As) and their isoelectronic equivalents (BN)12X4. *Chemical Physics Letters*, **1994**, 225, 448-453	2.5	21
51	On the Question of the Total Energy in the Fermi-L□wdin Orbital Self-Interaction Correction Method. *Journal of Chemical Theory and Computation*, **2018**, 14, 4122-4128	6.4	20

50	Atomistic dipole moments and polarizabilities of Na(N) clusters, N = 2-20. *Journal of Chemical Physics*, **2008**, 129, 144309	3.9	20
49	Photoelectron spectroscopy as a structural probe of intermediate size clusters. *Journal of Chemical Physics*, **2005**, 123, 204312	3.9	20
48	Enhanced stabilization of C60 crystals through doping. *Physical Review B*, **1992**, 45, 6919-6922	3.3	20
47	First-principles calculations of defect-induced lattice relaxation in ionic systems. *Physical Review B*, **1991**, 43, 2364-2371	3.3	18
46	Theoretical electronic structure studies of diamond: surfaces, adsorbates, defects and heterointerfaces. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology* , **1992**, 14, 87-92	3.1	17
45	Ground and excited states of the NaCl:Cu+ impurity system. *Physical Review B*, **1988**, 38, 12171-12183	3.3	17
44	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. II. Gauge consistency of the energy density at three levels of approximation. *Journal of Chemical Physics*, **2020**, 152, 214109	3.9	16
43	The interaction of ammonia with small iron clusters: infrared spectra and density functional calculations of Fen(NH3)m and Fen(ND3)m complexes. *Chemical Physics*, **2000**, 262, 41-51	2.3	16
42	Interpretation and Automatic Generation of Fermi-Orbital Descriptors. *Journal of Computational Chemistry*, **2019**, 40, 2843-2857	3.5	15
41	The effect of geometry on cluster polarizability: studies of sodium, copper, and silicon clusters at shape-transition sizes. *Journal of Chemical Physics*, **2011**, 134, 234505	3.9	15
40	Investigating the metallic behavior of Na clusters using site-specific polarizabilities. *Physical Review B*, **2014**, 89,	3.3	14
39	Chain formation and the origin of structure in the Raman spectrum of a□SiSe2. *Physical Review B*, **2001**, 65,	3.3	14
38	A study of substitutional nitrogen impurities in chemical vapor deposited diamond. *Journal of Applied Physics*, **1998**, 83, 4642-4646	2.5	14
37	Study of self-interaction errors in density functional predictions of dipole polarizabilities and ionization energies of water clusters using Perdew-Zunger and locally scaled self-interaction corrected methods. *Journal of Chemical Physics*, **2020**, 153, 164304	3.9	14
36	H2 saturation on palladium clusters. *Journal of Physical Chemistry A*, **2015**, 119, 3594-603	2.8	13
35	Chemical alloying and light-induced collapse of intermediate phases in chalcohalide glasses. *Journal of Physics Condensed Matter*, **2007**, 19, 226201	1.8	12
34	Analytic atomic gradients in the fermi-l□wdin orbital self-interaction correction. *Journal of Computational Chemistry*, **2019**, 40, 820-825	3.5	12
33	Statistical evaluation of the big bang search algorithm. *Computational Materials Science*, **2006**, 35, 232-237	3.2	11

32	Theory of the electronic states and absorption spectrum of the LiCl:Ag+ impurity system. *Physical Review B*, **1990**, 41, 947-957	3.3	11
31	Site specific atomic polarizabilities in endohedral fullerenes and carbon onions. *Journal of Chemical Physics*, **2015**, 143, 084306	3.9	9
30	Modeling the 119Sn M□ssbauer spectra of chalcogenide glasses using density-functional theory calculations. *Physical Review B*, **2002**, 65,	3.3	9
29	The Fermi-L□wdin self-interaction correction for ionization energies of organic molecules. *Journal of Chemical Physics*, **2020**, 153, 184303	3.9	9
28	Application of Self-Interaction Corrected Density Functional Theory to Early, Middle, and Late Transition States. *Journal of Physical Chemistry A*, **2020**, 124, 8223-8234	2.8	8
27	Viscous and nonviscous models of the partially filled rolling can. *American Journal of Physics*, **1996**, 64, 277-282	0.7	7
26	Self-interaction correction in water-ion clusters. *Journal of Chemical Physics*, **2021**, 154, 094302	3.9	6
25	How well do self-interaction corrections repair the overestimation of static polarizabilities in density functional calculations?. *Physical Chemistry Chemical Physics*, **2021**, 23, 18678-18685	3.6	6
24	Localization of excess electrons in cubic NanClm clusters. *Physical Review B*, **1992**, 45, 1927-1930	3.3	5
23	Multiplet-dependent wave functions from the local-spin-density approximation with self-interaction correction. *Physical Review B*, **1989**, 39, 1557-1563	3.3	5
22	Study of self-interaction-errors in barrier heights using locally scaled and Perdew-Zunger self-interaction methods.. *Journal of Chemical Physics*, **2022**, 156, 014306	3.9	5
21	Exploring and enhancing the accuracy of interior-scaled Perdew-Zunger self-interaction correction. *Journal of Chemical Physics*, **2021**, 154, 094105	3.9	5
20	Si clusters are more metallic than bulk Si. *Journal of Chemical Physics*, **2016**, 145, 244302	3.9	5
19	Signature of shape transition and shape coexistence in mesoscopic systems. *Chemical Physics Letters*, **2006**, 427, 147-152	2.5	4
18	Accuracy of density functional theory methods for the calculation of magnetic exchange couplings in binuclear iron(III) complexes. *Polyhedron*, **2020**, 176, 114194	2.7	4
17	Electronic structure of mononuclear Cu-based molecule from density-functional theory with self-interaction correction. *Journal of Chemical Physics*, **2021**, 155, 014106	3.9	4
16	Density-related properties from self-interaction corrected density functional theory calculations. *Journal of Chemical Physics*, **2021**, 154, 024102	3.9	4
15	Site-specific polarizabilities as predictors of favorable adsorption sites on Nan clusters. *Chemical Physics Letters*, **2011**, 503, 80-85	2.5	3

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14	Electronic properties of the eletride-type molecule Li(9-crown-3)2. Comparison of Hartree-Fock and local density approximations: implications for crystalline crown ether electrides. *Chemical Physics Letters*, **1996**, 262, 207-212	2.5	3
13	Shape of Small Silicon Clusters. *Physical Review Letters*, **1993**, 71, 2354-2354	7.4	3
12	Local Spin Density Treatment of Substitutional Defects in Ionic Crystals with Self-Interaction Corrections. *Advances in Atomic, Molecular and Optical Physics*, **2015**, 64, 15-27	1.7	2
11	Adsorption of Hydrocarbon Radicals on the Hydrogenated Diamond Surface. *Materials Research Society Symposia Proceedings*, **1989**, 162, 91		2
10	Initial Fermi orbital descriptors for FLOSIC calculations: The quick-FOD method. *Chemical Physics Letters*, **2021**, 780, 138952	2.5	2
9	Complex Fermi-L"{o}wdin orbital Self-interaction correction. *Journal of Chemical Physics*,	3.9	2
8	Comment on "Additional Insights Between Fermi-L□wdin Orbital SIC and the Localization Equation Constraints in SIC-DFT". *Journal of Physical Chemistry A*, **2019**, 123, 4322-4323	2.8	1
7	Forces and Geometry Optimization in First-Principles Atomic Cluster Calculations. *Materials Research Society Symposia Proceedings*, **1990**, 193, 107		1
6	Universality in size-driven evolution towards bulk polarizability of metals. *Nanoscale*, **2018**, 10, 17534-17539	7.7	1
5	Accurate Intramolecular Forces Within Gaussian Orbital Local-Density Framework: Progress Towards Real Dynamics **1991**, 231-245		1
4	Fermi-L□wdin orbital self-interaction correction of adsorption energies on transition metal ions.. *Journal of Chemical Physics*, **2022**, 156, 134102	3.9	1
3	Site-specific polarizabilities from analytic linear-response theory. *Chemical Physics Letters*, **2014**, 608, 24-27	2.5	
2	Nitrogen and Phosphorous Impurities in Diamond. *Materials Research Society Symposia Proceedings*, **1989**, 163, 89		
1	Growth of Silicon Nanoclusters **2004**, 83-96		