Koblar Alan Jackson

List of Publications by Year
in descending order

106	27,126	94269 37	31759 101
papers	citations	h-index	g-index

108	108	108	17718
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation. Physical Review B, 1992, 46, 6671-6687.	1.1	19,217
2	Variational mesh for quantum-mechanical simulations. Physical Review B, 1990, 41, 7453-7461.	1.1	484
3	Accurate forces in a local-orbital approach to the local-density approximation. Physical Review B, 1990, 42, 3276-3281.	1.1	348
4	Single-Parent Evolution Algorithm and the Optimization of Si Clusters. Physical Review Letters, 2000, 85, 546-549.	2.9	189
5	Raman-active modes ofaâˆ'GeSe2andaâˆ'GeS2:A first-principles study. Physical Review B, 1999, 60, R14985-R14989.	1.1	188
6	Shape of small silicon clusters. Physical Review Letters, 1993, 71, 727-730.	2.9	174
7	Unraveling the Shape Transformation in Silicon Clusters. Physical Review Letters, 2004, 93, .	2.9	150
8	Pseudoenergies for simulations on metallic systems. Physical Review B, 1991, 43, 7312-7315.	1.1	144
9	Theory of magnetic and structural ordering in iron clusters. Physical Review B, 1991, 44, 6558-6561.	1.1	101
10	Structure and shape variations in intermediate-size copper clusters. Journal of Chemical Physics, 2006, 124, 024308.	1.2	100
11	Zr@Si20: a strongly bound Si endohedral system. Chemical Physics Letters, 1996, 254, 249-256.	1.2	99
12	Structure and vibrational spectra of low-energy silicon clusters. Physical Review A, 1997, 56, 4890-4898.	1.0	90
13	First-principles study of the structural and electronic properties of Cu clusters. Physical Review B, 1993, 47, 9715-9722.	1.1	81
14	Scanning the potential energy surface of iron clusters: A novel search strategy. Journal of Chemical Physics, 2002, 116, 3576-3587.	1.2	74
15	Calculated polarizabilities of intermediate-size Si clusters. Physical Review A, 1999, 59, 3685-3689.	1.0	73
16	Density-functional-based predictions of Raman and IR spectra for small Si clusters. Physical Review B, 1997, 55, 2549-2555.	1.1	71
17	Vibrational frequencies and intensities of small molecules: All-electron, pseudopotential, and mixed-potential methodologies. Physical Review B, 1998, 58, 1786-1793.	1.1	70
18	First-principles study of intermediate size silver clusters: Shape evolution and its impact on cluster properties. Journal of Chemical Physics, 2006, 125, 144308.	1.2	67

#	Article	IF	Citations
19	Optical absorption spectra of intermediate-size silver clusters from first principles. Physical Review B, 2008, 78, .	1.1	67
20	Sharp Rigid to Floppy Phase Transition Induced by Dangling Ends in a Network Glass. Physical Review Letters, 2001, 87, .	2.9	64
21	Shape transition of medium-sized neutral silicon clusters. Physica Status Solidi (B): Basic Research, 2003, 240, 537-548.	0.7	62
22	Assessing student written problem solutions: A problem-solving rubric with application to introductory physics. Physical Review Physics Education Research, 2016, 12, .	1.4	60
23	Local-density-approximation-based simulations of hydrocarbon interactions with applications to diamond chemical vapor deposition. Physical Review B, 1991, 44, 3891-3899.	1.1	59
24	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.	3.3	57
25	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. Journal of Chemical Physics, 2019, 151, 214108.	1.2	56
26	Bonding of Endohedral Atoms in Small Carbon Fullerenes. The Journal of Physical Chemistry, 1994, 98, 7805-7810.	2.9	51
27	Donor levels and impurity-atom relaxation in nitrogen- and phosphorus-doped diamond. Physical Review B, 1990, 41, 12641-12649.	1.1	48
28	Stretched or noded orbital densities and self-interaction correction in density functional theory. Journal of Chemical Physics, 2019, 150, 174102.	1.2	46
29	Site-Specific Analysis of Dielectric Properties of Finite Systems. Journal of Physical Chemistry C, 2007, 111, 17952-17960.	1.5	45
30	First-principles absorption spectra of Cu<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mi>n</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math>(<mml:math) Tj ETQq0 0 0 rgBT /Overlock	1.1	45
31	The self-organized phase of bulk P x Se 1 â˜' x glasses. Europhysics Letters, 2003, 62, 49-55.	0.7	42
32	Vibrational signatures for low-energy intermediate-sized Si clusters. Physical Review B, 1996, 54, 2863-2867.	1.1	39
33	Self-consistent self-interaction corrected density functional theory calculations for atoms using Fermi-LÃ¶wdin orbitals: Optimized Fermi-orbital descriptors for Liâ€“Kr. Journal of Chemical Physics, 2017, 147, 164107.	1.2	39
34	Hydrogenated and deuterated iron clusters: Infrared spectra and density functional calculations. Journal of Chemical Physics, 1998, 109, 10692-10700.	1.2	38
35	Fermi-LÃ¶wdin orbital self-interaction correction using the strongly constrained and appropriately normed meta-GGA functional. Journal of Chemical Physics, 2019, 151, 154105.	1.2	38
36	Ball-and-Chain Dimers from a Hot Fullerene Plasma. Journal of Physical Chemistry A, 1999, 103, 5275-5284.	1.1	37

#	Article	IF	Citations
37	Electronic states of group-IV endohedral atoms inC28. Physical Review B, 1993, 48, 17556-17561.	1.1	36
38	H₂ Reactions on Palladium Clusters. Journal of Physical Chemistry A, 2013, 117, 10407-10415.	1.1	35
39	Structural growth behavior and polarizability of CdnTenâ€ˆ(n=1â€“14) clusters. Journal of Chemical Physics, 2009, 130, 214307.	1.2	34
40	Structure and energetics of SinNm clusters: Growth pathways in a heterogenous cluster system. Journal of Chemical Physics, 2000, 112, 1295-1305.	1.2	33
41	Fermi-LÃ¶wdin orbital self-interaction correction to magnetic exchange couplings. Journal of Chemical Physics, 2018, 149, 164101.	1.2	33
42	New theoretical model for the diamond 1score exciton. Physical Review Letters, 1991, 67, 2521-2524.	2.9	32
43	First-principles investigations of the polarizability of small-sized and intermediate-sized copper clusters. Journal of Chemical Physics, 2005, 122, 184317.	1.2	32
44	Icosahedral to double-icosahedral shape transition of copper clusters. Journal of Chemical Physics, 2012, 136, 104501.	1.2	32
45	Importance of self-interaction-error removal in density functional calculations on water cluster anions. Physical Chemistry Chemical Physics, 2020, 22, 3789-3799.	1.3	32
46	Shrinking Self-Interaction Errors with the Fermiâ€“LÃ¶wdin Orbital Self-Interaction-Corrected Density Functional Approximation. Journal of Physical Chemistry A, 2018, 122, 9307-9315.	1.1	30
47	The effect of self-interaction error on electrostatic dipoles calculated using density functional theory. Journal of Chemical Physics, 2019, 151, 174106.	1.2	29
48	Theoretical Investigation of Adsorption of Molecular Oxygen on Small Copper Clusters. Journal of Physical Chemistry A, 2011, 115, 8705-8712.	1.1	28
49	Self-interaction-free electric dipole polarizabilities for atoms and their ions using the Fermi-LÃ¶wdin self-interaction correction. Physical Review A, 2019, 100, .	1.0	27
50	A step in the direction of resolving the paradox of Perdewâ€“Zunger self-interaction correction. II. Gauge consistency of the energy density at three levels of approximation. Journal of Chemical Physics, 2020, 152, 214109.	1.2	23
51	Theoretical study of passivated small fullerenes C24X4 (Xî—»N, P, As) and their isoelectronic equivalents (BN)12X4. Chemical Physics Letters, 1994, 225, 448-453.	1.2	22
52	First-principles absorption spectra ofSin(n=20â€“28)clusters: Time-dependent local-density approximation versus predictions from Mie theory. Physical Review B, 2006, 74, .	1.1	22
53	On the Question of the Total Energy in the Fermiâ€“LÃ¶wdin Orbital Self-Interaction Correction Method. Journal of Chemical Theory and Computation, 2018, 14, 4122-4128.	2.3	22
54	Cage-forming tendencies in SinNm clusters. Chemical Physics Letters, 1998, 292, 235-242.	1.2	21

#	Article	IF	Citations
55	Photoelectron spectroscopy as a structural probe of intermediate size clusters. Journal of Chemical Physics, 2005, 123, 204312.	1.2	21
56	Atomistic dipole moments and polarizabilities of NaN clusters, N=2â€“20. Journal of Chemical Physics, 2008, 129, 144309.	1.2	21
57	Interpretation and Automatic Generation of Fermiâ€Orbital Descriptors. Journal of Computational Chemistry, 2019, 40, 2843-2857.	1.5	21
58	Study of self-interaction errors in density functional predictions of dipole polarizabilities and ionization energies of water clusters using Perdewâ€“Zunger and locally scaled self-interaction corrected methods. Journal of Chemical Physics, 2020, 153, 164304.	1.2	21
59	Enhanced stabilization ofC60crystals through doping. Physical Review B, 1992, 45, 6919-6922.	1.1	20
60	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.	1.7	20
61	First-principles calculations of defect-induced lattice relaxation in ionic systems. Physical Review B, 1991, 43, 2364-2371.	1.1	18
62	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.	0.9	18
63	Accuracy of density functional theory methods for the calculation of magnetic exchange couplings in binuclear iron(III) complexes. Polyhedron, 2020, 176, 114194.	1.0	18
64	Ground and excited states of the NaCl:Cu+impurity system. Physical Review B, 1988, 38, 12171-12183.	1.1	17
65	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.	1.2	17
66	H₂ Saturation on Palladium Clusters. Journal of Physical Chemistry A, 2015, 119, 3594-3603.	1.1	17
67	A study of substitutional nitrogen impurities in chemical vapor deposited diamond. Journal of Applied Physics, 1998, 83, 4642-4646.	1.1	16
68	Chain formation and the origin of structure in the Raman spectrum ofaâ^'SiSe2. Physical Review B, 2001, 65, .	1.1	16
69	Investigating the metallic behavior of Na clusters using site-specific polarizabilities. Physical Review B, 2014, 89, .	1.1	16
70	Analytic atomic gradients in the fermiâ€Ã¶wdin orbital selfâ€interaction correction. Journal of Computational Chemistry, 2019, 40, 820-825.	1.5	16
71	Self-interaction correction in waterâ€“ion clusters. Journal of Chemical Physics, 2021, 154, 094302.	1.2	16
72	How well do self-interaction corrections repair the overestimation of static polarizabilities in density functional calculations?. Physical Chemistry Chemical Physics, 2021, 23, 18678-18685.	1.3	14

#	Article	IF	Citations
73	Statistical evaluation of the big bang search algorithm. Computational Materials Science, 2006, 35, 232-237.	1.4	13
74	Viscous and nonviscous models of the partially filled rolling can. American Journal of Physics, 1996, 64, 277-282.	0.3	12
75	Chemical alloying and light-induced collapse of intermediate phases in chalcohalide glasses. Journal of Physics Condensed Matter, 2007, 19, 226201.	0.7	12
76	The Fermiâ€“LÃ¶wdin self-interaction correction for ionization energies of organic molecules. Journal of Chemical Physics, 2020, 153, 184303.	1.2	12
77	Application of Self-Interaction Corrected Density Functional Theory to Early, Middle, and Late Transition States. Journal of Physical Chemistry A, 2020, 124, 8223-8234.	1.1	12
78	Exploring and enhancing the accuracy of interior-scaled Perdewâ€“Zunger self-interaction correction. Journal of Chemical Physics, 2021, 154, 094105.	1.2	12
79	Electronic structure of mononuclear Cu-based molecule from density-functional theory with self-interaction correction. Journal of Chemical Physics, 2021, 155, 014106.	1.2	12
80	Study of self-interaction-errors in barrier heights using locally scaled and Perdewâ€“Zunger self-interaction methods. Journal of Chemical Physics, 2022, 156, 014306.	1.2	12
81	Theory of the electronic states and absorption spectrum of the LiCl:Ag+impurity system. Physical Review B, 1990, 41, 947-957.	1.1	11
82	Modeling the119SnMÃ¶ssbauer spectra of chalcogenide glasses using density-functional theory calculations. Physical Review B, 2002, 65, .	1.1	11
83	Site specific atomic polarizabilities in endohedral fullerenes and carbon onions. Journal of Chemical Physics, 2015, 143, 084306.	1.2	11
84	Si clusters are more metallic than bulk Si. Journal of Chemical Physics, 2016, 145, 244302.	1.2	11
85	Density-related properties from self-interaction corrected density functional theory calculations. Journal of Chemical Physics, 2021, 154, 024102.	1.2	8
86	Multiplet-dependent wave functions from the local-spin-density approximation with self-interaction correction. Physical Review B, 1989, 39, 1557-1563.	1.1	5
87	Localization of excess electrons in cubicNanClmclusters. Physical Review B, 1992, 45, 1927-1930.	1.1	5
88	Signature of shape transition and shape coexistence in mesoscopic systems. Chemical Physics Letters, 2006, 427, 147-152.	1.2	5
89	Interlayer polarizability in twisted bilayer graphene quantum dots. Physical Review B, 2021, 104, .	1.1	5
90	Complex Fermiâ€“LÃ¶wdin orbital self-interaction correction. Journal of Chemical Physics, 2022, 156, .	1.2	5

#	Article	IF	Citations
91	Shape of Small Silicon Clusters. Physical Review Letters, 1993, 71, 2354-2354.	2.9	4
92	Site-specific polarizabilities as predictors of favorable adsorption sites on Nan clusters. Chemical Physics Letters, 2011, 503, 80-85.	1.2	4
93	Initial Fermi orbital descriptors for FLOSIC calculations: The quick-FOD method. Chemical Physics Letters, 2021, 780, 138952.	1.2	4
94	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.	1.2	3
95	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.	2.3	3
96	Adsorption of Hydrocarbon Radicals on the Hydrogenated Diamond Surface. Materials Research Society Symposia Proceedings, 1989, 162, 91.	0.1	2
97	Universality in size-driven evolution towards bulk polarizability of metals. Nanoscale, 2018, 10, 17534-17539.	2.8	2
98	Fermiâ€“LÃ¶wdin orbital self-interaction correction of adsorption energies on transition metal ions. Journal of Chemical Physics, 2022, 156, 134102.	1.2	2
99	Forces and Geometry Optimization in First-Principles Atomic Cluster Calculations. Materials Research Society Symposia Proceedings, 1990, 193, 107.	0.1	1
100	Comment on â€œAdditional Insights Between Fermi-LÃ¶wdin Orbital SIC and the Localization Equation Constraints in SIC-DFTâ€• Journal of Physical Chemistry A, 2019, 123, 4322-4323.	1.1	1
101	Accurate Intramolecular Forces Within Gaussian Orbital Local-Density Framework: Progress Towards Real Dynamics. , 1991, , 231-245.		1
102	Nitrogen and Phosphorous Impurities in Diamond. Materials Research Society Symposia Proceedings, 1989, 163, 89.	0.1	0
103	Energetics and geometries for hydrocarbon radicals on the diamond surface. Carbon, 1990, 28, 801.	5.4	0
104	Shape Transition and Shape Coexistence in Atomic Clusters and Nuclei. AIP Conference Proceedings, 2005, , .	0.3	0
105	Site-specific polarizabilities from analytic linear-response theory. Chemical Physics Letters, 2014, 608, 24-27.	1.2	0
106	Growth of Silicon Nanoclusters. , 2004, , 83-96.		0