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	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
2	Fermiâ€“LÃ¶wdin orbital self-interaction correction of adsorption energies on transition metal ions. Journal of Chemical Physics, 2022, 156, 134102.	1.2	2
3	Complex Fermiâ€“LÃ¶wdin orbital self-interaction correction. Journal of Chemical Physics, 2022, 156, .	1.2	5
4	Density-related properties from self-interaction corrected density functional theory calculations. Journal of Chemical Physics, 2021, 154, 024102.	1.2	8
5	Self-interaction correction in waterâ€“ion clusters. Journal of Chemical Physics, 2021, 154, 094302.	1.2	16
6	Exploring and enhancing the accuracy of interior-scaled Perdewâ€“Zunger self-interaction correction. Journal of Chemical Physics, 2021, 154, 094105.	1.2	12
7	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
8	Initial Fermi orbital descriptors for FLOSIC calculations: The quick-FOD method. Chemical Physics Letters, 2021, 780, 138952.	1.2	4
9	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
10	Interlayer polarizability in twisted bilayer graphene quantum dots. Physical Review B, 2021, 104, .	1.1	5
11	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
12	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
13	The Fermiâ€“LÃ¶wdin self-interaction correction for ionization energies of organic molecules. Journal of Chemical Physics, 2020, 153, 184303.	1.2	12
14	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
15	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
16	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
17	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
18	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

#	Article	IF	Citations
19	Interpretation and Automatic Generation of Fermiâ€Orbital Descriptors. Journal of Computational Chemistry, 2019, 40, 2843-2857.	1.5	21
20	The effect of self-interaction error on electrostatic dipoles calculated using density functional theory. Journal of Chemical Physics, 2019, 151, 174106.	1.2	29
21	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
22	Stretched or noded orbital densities and self-interaction correction in density functional theory. Journal of Chemical Physics, 2019, 150, 174102.	1.2	46
23	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
24	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
25	Analytic atomic gradients in the fermiâ€LÃ¶wdin orbital selfâ€interaction correction. Journal of Computational Chemistry, 2019, 40, 820-825.	1.5	16
26	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
27	Fermi-LÃ¶wdin orbital self-interaction correction to magnetic exchange couplings. Journal of Chemical Physics, 2018, 149, 164101.	1.2	33
28	Universality in size-driven evolution towards bulk polarizability of metals. Nanoscale, 2018, 10, 17534-17539.	2.8	2
29	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
30	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
31	Si clusters are more metallic than bulk Si. Journal of Chemical Physics, 2016, 145, 244302.	1.2	11
32	Assessing student written problem solutions: A problem-solving rubric with application to introductory physics. Physical Review Physics Education Research, 2016, 12, .	1.4	60
33	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
34	H₂ Saturation on Palladium Clusters. Journal of Physical Chemistry A, 2015, 119, 3594-3603.	1.1	17
35	Site specific atomic polarizabilities in endohedral fullerenes and carbon onions. Journal of Chemical Physics, 2015, 143, 084306.	1.2	11
36	Investigating the metallic behavior of Na clusters using site-specific polarizabilities. Physical Review B, 2014, 89, .	1.1	16

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37	Site-specific polarizabilities from analytic linear-response theory. Chemical Physics Letters, 2014, 608, 24-27.	1.2	0
38	H₂ Reactions on Palladium Clusters. Journal of Physical Chemistry A, 2013, 117, 10407-10415.	1.1	35
39	Icosahedral to double-icosahedral shape transition of copper clusters. Journal of Chemical Physics, 2012, 136, 104501.	1.2	32
40	Theoretical Investigation of Adsorption of Molecular Oxygen on Small Copper Clusters. Journal of Physical Chemistry A, 2011, 115, 8705-8712.	1.1	28
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.	1.2	17
42	Site-specific polarizabilities as predictors of favorable adsorption sites on Nan clusters. Chemical Physics Letters, 2011, 503, 80-85.	1.2	4
43	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 ETQq1 1 0.784314 rgBT /O	1.1	45
44	Structural growth behavior and polarizability of CdnTenâ€ˆ(n=1â€“14) clusters. Journal of Chemical Physics, 2009, 130, 214307.	1.2	34
45	Atomistic dipole moments and polarizabilities of NaN clusters, N=2â€“20. Journal of Chemical Physics, 2008, 129, 144309.	1.2	21
46	Optical absorption spectra of intermediate-size silver clusters from first principles. Physical Review B, 2008, 78, .	1.1	67
47	Chemical alloying and light-induced collapse of intermediate phases in chalcohalide glasses. Journal of Physics Condensed Matter, 2007, 19, 226201.	0.7	12
48	Site-Specific Analysis of Dielectric Properties of Finite Systems. Journal of Physical Chemistry C, 2007, 111, 17952-17960.	1.5	45
49	Structure and shape variations in intermediate-size copper clusters. Journal of Chemical Physics, 2006, 124, 024308.	1.2	100
50	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
51	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
52	Statistical evaluation of the big bang search algorithm. Computational Materials Science, 2006, 35, 232-237.	1.4	13
53	Signature of shape transition and shape coexistence in mesoscopic systems. Chemical Physics Letters, 2006, 427, 147-152.	1.2	5
54	Shape Transition and Shape Coexistence in Atomic Clusters and Nuclei. AIP Conference Proceedings, 2005, , .	0.3	0

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55	First-principles investigations of the polarizability of small-sized and intermediate-sized copper clusters. Journal of Chemical Physics, 2005, 122, 184317.	1.2	32
56	Photoelectron spectroscopy as a structural probe of intermediate size clusters. Journal of Chemical Physics, 2005, 123, 204312.	1.2	21
57	Unraveling the Shape Transformation in Silicon Clusters. Physical Review Letters, 2004, 93, .	2.9	150
58	Growth of Silicon Nanoclusters. , 2004, , 83-96.		0
59	Shape transition of medium-sized neutral silicon clusters. Physica Status Solidi (B): Basic Research, 2003, 240, 537-548.	0.7	62
60	The self-organized phase of bulk P x Se 1 â^' x glasses. Europhysics Letters, 2003, 62, 49-55.	0.7	42
61	Modeling the119SnMÃ¶ssbauer spectra of chalcogenide glasses using density-functional theory calculations. Physical Review B, 2002, 65, .	1.1	11
62	Scanning the potential energy surface of iron clusters: A novel search strategy. Journal of Chemical Physics, 2002, 116, 3576-3587.	1.2	74
63	Chain formation and the origin of structure in the Raman spectrum ofaâ^'SiSe2. Physical Review B, 2001, 65, .	1.1	16
64	Sharp Rigid to Floppy Phase Transition Induced by Dangling Ends in a Network Glass. Physical Review Letters, 2001, 87, .	2.9	64
65	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
66	Structure and energetics of SinNm clusters: Growth pathways in a heterogenous cluster system. Journal of Chemical Physics, 2000, 112, 1295-1305.	1.2	33
67	Single-Parent Evolution Algorithm and the Optimization of Si Clusters. Physical Review Letters, 2000, 85, 546-549.	2.9	189
68	Calculated polarizabilities of intermediate-size Si clusters. Physical Review A, 1999, 59, 3685-3689.	1.0	73
69	Raman-active modes ofaâ^'GeSe2andaâ^'GeS2:A first-principles study. Physical Review B, 1999, 60, R14985-R14989.	1.1	188
70	Ball-and-Chain Dimers from a Hot Fullerene Plasma. Journal of Physical Chemistry A, 1999, 103, 5275-5284.	1.1	37
71	Cage-forming tendencies in SinNm clusters. Chemical Physics Letters, 1998, 292, 235-242.	1.2	21
72	A study of substitutional nitrogen impurities in chemical vapor deposited diamond. Journal of Applied Physics, 1998, 83, 4642-4646.	1.1	16

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73	Hydrogenated and deuterated iron clusters: Infrared spectra and density functional calculations. Journal of Chemical Physics, 1998, 109, 10692-10700.	1.2	38
74	Vibrational frequencies and intensities of small molecules: All-electron, pseudopotential, and mixed-potential methodologies. Physical Review B, 1998, 58, 1786-1793.	1.1	70
75	Density-functional-based predictions of Raman and IR spectra for small Si clusters. Physical Review B, 1997, 55, 2549-2555.	1.1	71
76	Structure and vibrational spectra of low-energy silicon clusters. Physical Review A, 1997, 56, 4890-4898.	1.0	90
77	Viscous and nonviscous models of the partially filled rolling can. American Journal of Physics, 1996, 64, 277-282.	0.3	12
78	Zr@Si20: a strongly bound Si endohedral system. Chemical Physics Letters, 1996, 254, 249-256.	1.2	99
79	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
80	Vibrational signatures for low-energy intermediate-sized Si clusters. Physical Review B, 1996, 54, 2863-2867.	1.1	39
81	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
82	Bonding of Endohedral Atoms in Small Carbon Fullerenes. The Journal of Physical Chemistry, 1994, 98, 7805-7810.	2.9	51
83	First-principles study of the structural and electronic properties of Cu clusters. Physical Review B, 1993, 47, 9715-9722.	1.1	81
84	Electronic states of group-IV endohedral atoms inC28. Physical Review B, 1993, 48, 17556-17561.	1.1	36
85	Shape of Small Silicon Clusters. Physical Review Letters, 1993, 71, 2354-2354.	2.9	4
86	Shape of small silicon clusters. Physical Review Letters, 1993, 71, 727-730.	2.9	174
87	Enhanced stabilization ofC60crystals through doping. Physical Review B, 1992, 45, 6919-6922.	1.1	20
88	Localization of excess electrons in cubicNanClmclusters. Physical Review B, 1992, 45, 1927-1930.	1.1	5
89	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
90	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

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91	Theory of magnetic and structural ordering in iron clusters. Physical Review B, 1991, 44, 6558-6561.	1.1	101
92	Pseudoenergies for simulations on metallic systems. Physical Review B, 1991, 43, 7312-7315.	1.1	144
93	First-principles calculations of defect-induced lattice relaxation in ionic systems. Physical Review B, 1991, 43, 2364-2371.	1.1	18
94	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
95	New theoretical model for the diamond 1score exciton. Physical Review Letters, 1991, 67, 2521-2524.	2.9	32
96	Accurate Intramolecular Forces Within Gaussian Orbital Local-Density Framework: Progress Towards Real Dynamics. , 1991, , 231-245.		1
97	Forces and Geometry Optimization in First-Principles Atomic Cluster Calculations. Materials Research Society Symposia Proceedings, 1990, 193, 107.	0.1	1
98	Energetics and geometries for hydrocarbon radicals on the diamond surface. Carbon, 1990, 28, 801.	5.4	0
99	Donor levels and impurity-atom relaxation in nitrogen- and phosphorus-doped diamond. Physical Review B, 1990, 41, 12641-12649.	1.1	48
100	Accurate forces in a local-orbital approach to the local-density approximation. Physical Review B, 1990, 42, 3276-3281.	1.1	348
101	Variational mesh for quantum-mechanical simulations. Physical Review B, 1990, 41, 7453-7461.	1.1	484
102	Theory of the electronic states and absorption spectrum of the LiCl:Ag+impurity system. Physical Review B, 1990, 41, 947-957.	1.1	11
103	Multiplet-dependent wave functions from the local-spin-density approximation with self-interaction correction. Physical Review B, 1989, 39, 1557-1563.	1.1	5
104	Adsorption of Hydrocarbon Radicals on the Hydrogenated Diamond Surface. Materials Research Society Symposia Proceedings, 1989, 162, 91.	0.1	2
105	Nitrogen and Phosphorous Impurities in Diamond. Materials Research Society Symposia Proceedings, 1989, 163, 89.	0.1	0
106	Ground and excited states of the NaCl:Cu+impurity system. Physical Review B, 1988, 38, 12171-12183.	1.1	17