Mark R Pederson

List of Publications by Year
in descending order

70 papers	23,590 citations	136950 32 h-index	106344 65 g-index
70 all docs	70 docs citations	70 times ranked	17764 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.	3.2	19,217
2	Infrared intensities and Raman-scattering activities within density-functional theory. Physical Review B, 1996, 54, 7830-7836.	3.2	579
3	Variational mesh for quantum-mechanical simulations. Physical Review B, 1990, 41, 7453-7461.	3.2	484
4	Accurate forces in a local-orbital approach to the local-density approximation. Physical Review B, 1990, 42, 3276-3281.	3.2	348
5	Towards structureâ€“propertyâ€“function relationships for eumelanin. Soft Matter, 2006, 2, 37-44.	2.7	263
6	Optimization of Gaussian basis sets for density-functional calculations. Physical Review A, 1999, 60, 2840-2847.	2.5	250
7	Localâ€density Hartreeâ€“Fock theory of electronic states of molecules with selfâ€interaction correction. Journal of Chemical Physics, 1984, 80, 1972-1975.	3.0	198
8	Communication: Self-interaction correction with unitary invariance in density functional theory. Journal of Chemical Physics, 2014, 140, 121103.	3.0	168
9	Journal of Chemical Physics, 1985, 82, 2688-2699.	3.0	167
10	Pseudoenergies for simulations on metallic systems. Physical Review B, 1991, 43, 7312-7315.	3.2	144
11	Electron Attachment to a Negative Ion:e+C84â¯â‡ŒC84â¯2. Physical Review Letters, 1997, 78, 4367-4370.	7.8	110
12	Localized and canonical atomic orbitals in selfâ€interaction corrected local density functional approximation. Journal of Chemical Physics, 1988, 88, 1807-1817.	3.0	96
13	Density functional studies of molecular magnets. Physica Status Solidi (B): Basic Research, 2006, 243, 2533-2572.	1.5	95
14	Fermi orbital derivatives in self-interaction corrected density functional theory: Applications to closed shell atoms. Journal of Chemical Physics, 2015, 142, 064112.	3.0	78
15	Full self-consistency in the Fermi-orbital self-interaction correction. Physical Review A, 2017, 95, .	2.5	76
16	Hamiltonian of theV15Spin System from First-Principles Density-Functional Calculations. Physical Review Letters, 2001, 86, 3400-3403.	7.8	74
17	Magnetic and electronic properties of rhodium clusters. Physical Review A, 1998, 58, 2196-2202.	2.5	72
18	Vibrational frequencies and intensities of small molecules: All-electron, pseudopotential, and mixed-potential methodologies. Physical Review B, 1998, 58, 1786-1793.	3.2	70

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19	Density functional based studies of transition states and barriers for hydrogen exchange and abstraction reactions. Journal of Chemical Physics, 1995, 102, 9345-9349.	3.0	65
20	Density-functional theory calculation of the intermolecular exchange interaction in the magneticMn4dimer. Physical Review B, 2003, 68, .	3.2	60
21	Static dielectric response of icosahedral fullerenes from<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:math>to<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>2160</mml:mn></mml:msub></mml:math>characterized by	3.2	58
22	First-principles study of spin-electric coupling in a<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:mo>{</mml:mo><mml:mrow><mml:msub><mml:mrow><mml:mtext>Cu</mml:mtext></mml:mrow> molecular magnet. Physical Review B, 2010, 82, .	3.2	56
23	Properties of low-lying excited manifolds inMn12acetate. Physical Review B, 2004, 69, .	3.2	47
24	Effect of extra electrons on the exchange and magnetic anisotropy in the anionic single-molecule magnetMn12. Physical Review B, 2004, 70, .	3.2	47
25	Vibrational stability and electronic structure of a<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>B</mml:mtext><mml:mrow><mml:mn>80</mml:mn></mml:mrow></mml:mrow></mml:m Physical Review B, 2008, 78, .	3.2	47
26	Self-Interaction Corrections Within the Fermi-Orbital-Based Formalism. Advances in Atomic, Molecular and Optical Physics, 2015, 64, 153-180.	2.3	42
27	Many-body potential and structure for rhodium clusters. Journal of Chemical Physics, 2000, 112, 2301-2307.	3.0	39
28	Density-Functional-Based Determination of Vibrational Polarizabilities in Molecules within the Double-Harmonic Approximation:â€‰ Derivation and Application. Journal of Chemical Theory and Computation, 2005, 1, 590-596.	5.3	39
29	Magnetic ordering, electronic structure, and magnetic anisotropy energy in the high-spinMn10single molecule magnet. Physical Review B, 2002, 66, .	3.2	38
30	A theoretical study of rare-gas diatomic molecules with the generalized-gradient approximation to density functional theory. International Journal of Quantum Chemistry, 1998, 69, 619-627.	2.0	37
31	Fourth-Order Magnetic Anisotropy and Tunnel Splittings inMn12from Spin-Orbit-Vibron Interactions. Physical Review Letters, 2002, 89, 097202.	7.8	37
32	Self-interaction corrections applied to Mg-porphyrin, C60, and pentacene molecules. Journal of Chemical Physics, 2016, 144, 164117.	3.0	34
33	Electronic structure and magnetic anisotropy of the [Co4(hmp)4(CH3OH)4Cl4] molecule. Chemical Physics Letters, 2002, 360, 144-148.	2.6	32
34	Structural and bonding properties of bcc-based<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>B</mml:mtext><mml:mrow><mml:mn>80</mml:mn></mml:mrow></mml:mrow></mml:msu Physical Review B, 2008, 78, .	3.2	29
35	Fermi orbital self-interaction corrected electronic structure of molecules beyond local density approximation. Journal of Chemical Physics, 2015, 143, 224104.	3.0	29
36	Predicted infrared and Raman spectra for neutralTi8C12isomers. Physical Review A, 2002, 66, .	2.5	26

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37	Electronic-structure-based investigation of magnetism in the Fe[sub 8] molecular magnet. Journal of Applied Physics, 2002, 91, 7149.	2.5	26
38	Second-order transverse magnetic anisotropy induced by disorder in the single-molecule magnetMn12. Physical Review B, 2004, 69, .	3.2	25
39	Theoretical infrared, Raman, and optical spectra of theB36N36cage. Physical Review A, 2005, 71, .	2.5	24
40	A new density functional for fractionally occupied orbital systems with application to ionization and transition energies. Journal of Chemical Physics, 1987, 86, 258-267.	3.0	23
41	Density functional study of the conformers of Co4-based single-molecule magnet. International Journal of Quantum Chemistry, 2003, 93, 324-331.	2.0	23
42	Electronic structure and rebonding in the onionlikeAs@Ni12@As20cluster. Physical Review B, 2003, 68, .	3.2	21
43	Density-functional based determination of the CH3-CH4 hydrogen exchange reaction barrier. Chemical Physics Letters, 1994, 230, 54-60.	2.6	20
44	Molecular structures and vibrations of neutral and anionicCuOx(x=1â€“3,6)clusters. Physical Review A, 2004, 69, .	2.5	19
45	The Role of Self-Interaction Corrections, Vibrations, and Spin-Orbit in Determining the Ground Spin State in a Simple Heme. Magnetochemistry, 2017, 3, 31.	2.4	18
46	Reexamination of the Jahn-Teller instability inC6H6+andC6H6â^'. Physical Review A, 2005, 72, .	2.5	16
47	Self-interaction correction in waterâ€“ion clusters. Journal of Chemical Physics, 2021, 154, 094302.	3.0	16
48	Comparative study of unscreened and screened molecular static linear polarizability in the Hartreeâ€“Fock, hybridâ€density functional, and density functional models. International Journal of Quantum Chemistry, 2008, 108, 307-317.	2.0	14
49	Understanding the electronic structure, optical, and vibrational properties of theFe8Br8single-molecule magnet. Physical Review B, 2004, 70, .	3.2	13
50	Stability, electronic structure, and vibrational modes of theTi8C12dimer. Physical Review B, 2002, 66, .	3.2	11
51	Use of LÃ¶wdin orthogonalised Fermi orbitals for self-interaction corrections in an iron porphyrin. Molecular Physics, 2017, 115, 552-559.	1.7	11
52	A multiferroic molecular magnetic qubit. Journal of Chemical Physics, 2019, 151, 174105.	3.0	9
53	Incommensurate transverse anisotropy induced by disorder and spin-orbit-vibron coupling in Mn12 acetate. Journal of Applied Physics, 2005, 97, 10M505.	2.5	8
54	Magnetic Signatures of Hydroxylâ€•and Waterâ€Terminated Neutral and Tetraâ€Anionic Mn₁₂â€Acetate. Journal of Computational Chemistry, 2019, 40, 2301-2308.	3.3	8

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55	Symmetry Breaking within Fermiâ€“LÃ¶wdin Orbital Self-Interaction Corrected Density Functional Theory. Journal of Chemical Theory and Computation, 2017, 13, 5823-5828.	5.3	6
56	Electromagnetic control of spin ordered Mn₃ qubits: a density functional study. Physical Chemistry Chemical Physics, 2020, 22, 27547-27553.	2.8	5
57	Complex Fermiâ€“LÃ¶wdin orbital self-interaction correction. Journal of Chemical Physics, 2022, 156, .	3.0	5
58	Comparison of vibrational and electronic contributions to van der Waals interactions. Physical Review B, 2006, 73, .	3.2	3
59	Electronic control of strong magnetic anisotropy in Co-based single-molecule magnets. Physical Review B, 2021, 104, .	3.2	3
60	Studies of Large Lithium Clusters and their Vacancies with Highly Optimized Localized Orbitals. Materials Research Society Symposia Proceedings, 1988, 141, 153.	0.1	2
61	Adsorption of Hydrocarbon Radicals on the Hydrogenated Diamond Surface. Materials Research Society Symposia Proceedings, 1989, 162, 91.	0.1	2
62	Theoretical Investigation of Fluorinated and Hydrocenated Diamond <100> Filks. Materials Research Society Symposia Proceedings, 1992, 270, 389.	0.1	2
63	Electronic and magnetic signatures of low lying spin flip excitonic states of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si15.svg"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="normal">Mn</mml:mi></mml:mrow><mml:mrow><mml:mn>12</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>	0.2	2
64	Forces and Geometry Optimization in First-Principles Atomic Cluster Calculations. Materials Research Society Symposia Proceedings, 1990, 193, 107.	0.1	1
65	Communication: Practical and rigorous reduction of the many-electron quantum mechanical Coulomb problem to O(N2/3) storage. Journal of Chemical Physics, 2015, 142, 141102.	3.0	1
66	A theoretical study of rare-gas diatomic molecules with the generalized-gradient approximation to density functional theory. , 1998, 69, 619.		1
67	Density-Functional Based Investigation of Molecular Magnets. Computational Chemistry - Reviews of Current Trends, 2006, , 83-120.	0.4	1
68	Calculation of the Stability and the Polarizability of Isolated Fullerene Molecules as a Function of Charge State. Materials Research Society Symposia Proceedings, 1992, 270, 209.	0.1	0
69	Polarizabilities of intermediate sized lithium clusters from density-functional theory. Journal of Computational Methods in Sciences and Engineering, 2008, 7, 495-505.	0.2	0
70	ELECTRONIC STRUCTURE AND STABILITY OF THE As@Ni₁₂@As₂₀ AND As CAGES. , 2005, , .		0