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	Complex Fermiâ€“LÃ¶wdin orbital self-interaction correction. Journal of Chemical Physics, 2022, 156, .	3.0	5
2	Self-interaction correction in waterâ€“ion clusters. Journal of Chemical Physics, 2021, 154, 094302.	3.0	16
3	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>	2.2	2
4	Electronic control of strong magnetic anisotropy in Co-based single-molecule magnets. Physical Review B, 2021, 104, .	3.2	3
5	Electromagnetic control of spin ordered Mn₃ qubits: a density functional study. Physical Chemistry Chemical Physics, 2020, 22, 27547-27553.	2.8	5
6	Magnetic Signatures of Hydroxylâ€•and Waterâ€Terminated Neutral and Tetraâ€Anionic Mn₁₂â€Acetate. Journal of Computational Chemistry, 2019, 40, 2301-2308.	3.3	8
7	A multiferroic molecular magnetic qubit. Journal of Chemical Physics, 2019, 151, 174105.	3.0	9
8	Use of LÃ¶wdin orthogonalised Fermi orbitals for self-interaction corrections in an iron porphyrin. Molecular Physics, 2017, 115, 552-559.	1.7	11
9	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
10	Full self-consistency in the Fermi-orbital self-interaction correction. Physical Review A, 2017, 95, .	2.5	76
11	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
12	Self-interaction corrections applied to Mg-porphyrin, C60, and pentacene molecules. Journal of Chemical Physics, 2016, 144, 164117.	3.0	34
13	Fermi orbital self-interaction corrected electronic structure of molecules beyond local density approximation. Journal of Chemical Physics, 2015, 143, 224104.	3.0	29
14	Self-Interaction Corrections Within the Fermi-Orbital-Based Formalism. Advances in Atomic, Molecular and Optical Physics, 2015, 64, 153-180.	2.3	42
15	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
16	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
17	Communication: Self-interaction correction with unitary invariance in density functional theory. Journal of Chemical Physics, 2014, 140, 121103.	3.0	168
18	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> molecular magnet. Physical Review B, 2010, 82, .	3.2	56

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19	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
20	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 vibrational stability and electronic structure. Physical Review B, 2008, 77, .	3.2	58
21	Vibrational stability and electronic structure of<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:msub></mml:mrow></mml:math>. Physical Review B, 2008, 78, .	3.2	47
22	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:msub></mml:mrow></mml:math>. Physical Review B, 2008, 78, .	3.2	29
23	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
24	Towards structureâ€“propertyâ€“function relationships for eumelanin. Soft Matter, 2006, 2, 37-44.	2.7	263
25	Density functional studies of molecular magnets. Physica Status Solidi (B): Basic Research, 2006, 243, 2533-2572.	1.5	95
26	Comparison of vibrational and electronic contributions to van der Waals interactions. Physical Review B, 2006, 73, .	3.2	3
27	Density-Functional Based Investigation of Molecular Magnets. Computational Chemistry - Reviews of Current Trends, 2006, , 83-120.	0.4	1
28	Incommensurate transverse anisotropy induced by disorder and spin-orbit-vibron coupling in Mn12 acetate. Journal of Applied Physics, 2005, 97, 10M505.	2.5	8
29	Theoretical infrared, Raman, and optical spectra of theB36N36cage. Physical Review A, 2005, 71, .	2.5	24
30	Reexamination of the Jahn-Teller instability inC6H6+andC6H6â^'. Physical Review A, 2005, 72, .	2.5	16
31	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
32	ELECTRONIC STRUCTURE AND STABILITY OF THE As@Ni₁₂@As₂₀ AND As CAGES. , 2005, , .		0
33	Properties of low-lying excited manifolds inMn12acetate. Physical Review B, 2004, 69, .	3.2	47
34	Second-order transverse magnetic anisotropy induced by disorder in the single-molecule magnetMn12. Physical Review B, 2004, 69, .	3.2	25
35	Molecular structures and vibrations of neutral and anionicCuOx(x=1â€“3,6)clusters. Physical Review A, 2004, 69, .	2.5	19
36	Effect of extra electrons on the exchange and magnetic anisotropy in the anionic single-molecule magnetMn12. Physical Review B, 2004, 70, .	3.2	47

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37	Understanding the electronic structure, optical, and vibrational properties of theFe8Br8single-molecule magnet. Physical Review B, 2004, 70, .	3.2	13
38	Density functional study of the conformers of Co4-based single-molecule magnet. International Journal of Quantum Chemistry, 2003, 93, 324-331.	2.0	23
39	Density-functional theory calculation of the intermolecular exchange interaction in the magneticMn4dimer. Physical Review B, 2003, 68, .	3.2	60
40	Electronic structure and rebonding in the onionlikeAs@Ni12@As20cluster. Physical Review B, 2003, 68, .	3.2	21
41	Predicted infrared and Raman spectra for neutralTi8C12isomers. Physical Review A, 2002, 66, .	2.5	26
42	Fourth-Order Magnetic Anisotropy and Tunnel Splittings inMn12from Spin-Orbit-Vibron Interactions. Physical Review Letters, 2002, 89, 097202.	7.8	37
43	Magnetic ordering, electronic structure, and magnetic anisotropy energy in the high-spinMn10single molecule magnet. Physical Review B, 2002, 66, .	3.2	38
44	Stability, electronic structure, and vibrational modes of theTi8C12dimer. Physical Review B, 2002, 66, .	3.2	11
45	Electronic-structure-based investigation of magnetism in the Fe[sub 8] molecular magnet. Journal of Applied Physics, 2002, 91, 7149.	2.5	26
46	Electronic structure and magnetic anisotropy of the [Co4(hmp)4(CH3OH)4Cl4] molecule. Chemical Physics Letters, 2002, 360, 144-148.	2.6	32
47	Hamiltonian of theV15Spin System from First-Principles Density-Functional Calculations. Physical Review Letters, 2001, 86, 3400-3403.	7.8	74
48	Many-body potential and structure for rhodium clusters. Journal of Chemical Physics, 2000, 112, 2301-2307.	3.0	39
49	Optimization of Gaussian basis sets for density-functional calculations. Physical Review A, 1999, 60, 2840-2847.	2.5	250
50	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
51	Magnetic and electronic properties of rhodium clusters. Physical Review A, 1998, 58, 2196-2202.	2.5	72
52	Vibrational frequencies and intensities of small molecules: All-electron, pseudopotential, and mixed-potential methodologies. Physical Review B, 1998, 58, 1786-1793.	3.2	70
53	A theoretical study of rare-gas diatomic molecules with the generalized-gradient approximation to density functional theory. , 1998, 69, 619.		1
54	Electron Attachment to a Negative Ion:e+C84â^'â‡ŒC84â^'2. Physical Review Letters, 1997, 78, 4367-4370.	7.8	110

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55	Infrared intensities and Raman-scattering activities within density-functional theory. Physical Review B, 1996, 54, 7830-7836.	3.2	579
56	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
57	Density-functional based determination of the CH3-CH4 hydrogen exchange reaction barrier. Chemical Physics Letters, 1994, 230, 54-60.	2.6	20
58	Theoretical Investigation of Fluorinated and Hydrocenated Diamond <100> Filks. Materials Research Society Symposia Proceedings, 1992, 270, 389.	0.1	2
59	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
60	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
61	Pseudoenergies for simulations on metallic systems. Physical Review B, 1991, 43, 7312-7315.	3.2	144
62	Forces and Geometry Optimization in First-Principles Atomic Cluster Calculations. Materials Research Society Symposia Proceedings, 1990, 193, 107.	0.1	1
63	Accurate forces in a local-orbital approach to the local-density approximation. Physical Review B, 1990, 42, 3276-3281.	3.2	348
64	Variational mesh for quantum-mechanical simulations. Physical Review B, 1990, 41, 7453-7461.	3.2	484
65	Adsorption of Hydrocarbon Radicals on the Hydrogenated Diamond Surface. Materials Research Society Symposia Proceedings, 1989, 162, 91.	0.1	2
66	Localized and canonical atomic orbitals in selfâ€interaction corrected local density functional approximation. Journal of Chemical Physics, 1988, 88, 1807-1817.	3.0	96
67	Studies of Large Lithium Clusters and their Vacancies with Highly Optimized Localized Orbitals. Materials Research Society Symposia Proceedings, 1988, 141, 153.	0.1	2
68	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
69	Journal of Chemical Physics, 1985, 82, 2688-2699.	3.0	167
70	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