Hai-Ping Cheng

List of Publications by Year
in descending order

102	3,024	218677	168389
papers	citations	26 h-index	53 g-index

103	103	103	4179
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Coherent Electron Transport through an Azobenzene Molecule: A Light-Driven Molecular Switch. Physical Review Letters, 2004, 92, 158301.	7.8	249
2	Bulk Separative Enrichment in Metallic or Semiconducting Single-Walled Carbon Nanotubes. Nano Letters, 2003, 3, 1245-1249.	9.1	246
3	Proximity of antiferromagnetism and superconductivity in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LaFeAsO</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</m Effective Hamiltonian fromab initiostudies. Physical Review B, 2008, 77, .	3.2	245
4	Transition metal adatom and dimer adsorbed on graphene: Induced magnetization and electronic structures. Physical Review B, 2010, 81, .	3.2	234
5	Spin fluctuations and superconductivity in a three-dimensional tight-binding model for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BaFe</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml Physical Review B, 2010, 81, .	3.2	190
6	Absence of a Dirac cone in silicene on Ag(111): First-principles density functional calculations with a modified effective band structure technique. Physical Review B, 2013, 87, .	3.2	141
7	Oxygen Reduction Activity on Perovskite Oxide Surfaces: A Comparative First-Principles Study of LaMnO₃, LaFeO₃, and LaCrO₃. Journal of Physical Chemistry C, 2013, 117, 2106-2112.	3.1	140
8	Water Clusters:Â Fascinating Hydrogen-Bonding Networks, Solvation Shell Structures, and Proton Motion. Journal of Physical Chemistry A, 1998, 102, 6201-6204.	2.5	113
9	Current-voltage characteristics through a single light-sensitive molecule. Physical Review B, 2006, 73, .	3.2	87
10	Waterâ€“silica surface interactions: A combined quantum-classical molecular dynamic study of energetics and reaction pathways. Journal of Chemical Physics, 2003, 119, 6418-6422.	3.0	78
11	Electronic structure and spin-dependent tunneling conductance under a finite bias. Physical Review B, 2004, 69, .	3.2	66
12	Determining gap nodal structures in Fe-based superconductors: Theory of the angle dependence of the low-temperature specific heat in an applied magnetic field. Physical Review B, 2008, 77, .	3.2	47
13	The stability of free and oxidized silver clusters. Journal of Chemical Physics, 2003, 118, 10956-10962.	3.0	44
14	Two bonding configurations for individually adsorbed<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>C</mml:mtext><mml:mrow><mml:mn>60</mml:mn></mml:mrow></mml:msu on Au(111). Physical Review B, 2010, 82, .	3.2	42
15	Anisotropic quasiparticle lifetimes in Fe-based superconductors. Physical Review B, 2011, 83, .	3.2	37
16	Effects of strain and defects on the electron conductance of metallic carbon nanotubes. Physical Review B, 2007, 75, .	3.2	36
17	Doping effects of Se vacancies in monolayer FeSe. Physical Review B, 2014, 89, .	3.2	36
18	Unified interatomic potential and energy barrier distributions for amorphous oxides. Journal of Chemical Physics, 2013, 139, 154506.	3.0	35

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19	Molecular dynamics modeling of mechanical loss in amorphous tantala and titania-doped tantala. Physical Review B, 2016, 93, .	3.2	33
20	Decoherence in Molecular Electron Spin Qubits: Insights from Quantum Many-Body Simulations. Journal of Physical Chemistry Letters, 2020, 11, 2074-2078.	4.6	32
21	High Precision Detection of Change in Intermediate Range Order of Amorphous Zirconia-Doped Tantala Thin Films Due to Annealing. Physical Review Letters, 2019, 123, 045501.	7.8	29
22	Magnetoelectric behavior via a spin state transition. Nature Communications, 2019, 10, 4043.	12.8	29
23	First-principles study of Fe/MgO based magnetic tunnel junctions with Mg interlayers. Physical Review B, 2010, 82, .	3.2	28
24	Molecular analogue of the perovskite repeating unit and evidence for direct MnIII-CeIV-MnIII exchange coupling pathway. Nature Communications, 2017, 8, 500.	12.8	28
25	Application of Quantum Computing to Biochemical Systems: A Look to the Future. Frontiers in Chemistry, 2020, 8, 587143.	3.6	28
26	Ab Initio Calculation of a Graphene-Ribbon-Based Molecular Switch. Journal of Physical Chemistry C, 2007, 111, 14266-14273.	3.1	27
27	A quantum molecular dynamics study of the properties of NO+(H2O)n clusters. Journal of Chemical Physics, 1998, 108, 2015-2023.	3.0	23
28	All-electron self-consistent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:n the Matsubara-time domain: Implementation and benchmarks of semiconductors and insulators. Physical Review B, 2016, 93, .	3.2	23
29	Electronic and transport properties of azobenzene monolayer junctions as molecular switches. Physical Review B, 2012, 86, .	3.2	22
30	Two-dimensional lateral GaN/SiC heterostructures: First-principles studies of electronic and magnetic properties. Physical Review B, 2017, 95, .	3.2	22
31	Tailoring electrocatalytic activity of in situ crafted perovskite oxide nanocrystals via size and dopant control. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	22
32	Giant Magnetoelectric Coupling and Magnetic-Field-Induced Permanent Switching in a Spin Crossover Mn(III) Complex. Inorganic Chemistry, 2021, 60, 6167-6175.	4.0	21
33	Quantum-Inspired Algorithm for the Factorized Form of Unitary Coupled Cluster Theory. Journal of Chemical Theory and Computation, 2021, 17, 841-847.	5.3	21
34	First-principles studies of electric field effects on the electronic structure of trilayer graphene. Physical Review B, 2016, 94, .	3.2	20
35	Nonequilibrium Greenâ€™s function study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Pd</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:msu carbon nanotubes as hydrogen sensors. Physical Review B, 2009, 79, .	3.2	19
36	Perfect spin-filtering and giant magnetoresistance with Fe-terminated graphene nanoribbon. Applied Physics Letters, 2011, 99, .	3.3	19

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37	First-principles investigation of a monolayer ofC60onhâ˜BNâ•Ni(111). Physical Review B, 2005, 72, .	3.2	18
38	Insensitivity ofd-wave pairing to disorder in the high-temperature cuprate superconductors. Physical Review B, 2009, 79, .	3.2	18
39	Reversible Spin Polarization at Hybrid Organicâ€“Ferromagnetic Interfaces. Journal of Physical Chemistry Letters, 2013, 4, 3508-3512.	4.6	18
40	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>DFT</mml:mi><mml:mo>+</mml:mo><mml:mi>DMFT</m calculations of the complex band and tunneling behavior for the transition metal monoxides MnO, FeO, CoO, and NiO. Physical Review B, 2019, 100, .	3.2	18
41	Cluster-surface collisions: Characteristics of Xe55- and C20â€“Si[111] surface bombardment. Journal of Chemical Physics, 1999, 111, 7583-7592.	3.0	17
42	All-electron GW quasiparticle band structures of group 14 nitride compounds. Journal of Chemical Physics, 2014, 141, 044709.	3.0	17
43	Theoretical prediction of magnetic exchange coupling constants from broken-symmetry coupled cluster calculations. Journal of Chemical Physics, 2020, 152, 234115.	3.0	17
44	Transparent interface between classical molecular dynamics and first-principles molecular dynamics. International Journal of Quantum Chemistry, 2003, 93, 1-8.	2.0	16
45	Asymmetric Design of Spin-Crossover Complexes to Increase the Volatility for Surface Deposition. Journal of the American Chemical Society, 2021, 143, 14563-14572.	13.7	16
46	Water-silica interaction in clusters. European Physical Journal D, 2003, 24, 323-326.	1.3	15
47	Giant Molecular Magnetocapacitance. Physical Review Letters, 2013, 110, 217205.	7.8	15
48	First-principles simulations of a graphene-based field-effect transistor. Physical Review B, 2015, 91, .	3.2	15
49	Topological insulator-metal transition and molecular electronics device based on zigzag phagraphene nanoribbon. Journal of Applied Physics, 2018, 124, .	2.5	14
50	First-principles theory for Schottky barrier physics. Physical Review B, 2021, 104, .	3.2	14
51	OPAL: A multiscale multicenter simulation package based on MPIâ€2 protocol. International Journal of Quantum Chemistry, 2011, 111, 4020-4029.	2.0	13
52	Origin of the second peak in the mechanical loss function of amorphous silica. Physical Review B, 2017, 95, .	3.2	13
53	Single-molecule magnet<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Mn</mml:mi><mml:mn>12</mml:mn></mml:msub></mml:math>on graphene. Physical Review B, 2014, 90, .	3.2	12
54	Electron transport in graphene/graphene side-contact junction by plane-wave multiple-scattering method. Physical Review B, 2015, 91, .	3.2	12

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55	Long-Range Ferromagnetic Exchange Interactions Mediated by Mnâ€“Ce^{IV}â€“Mn Superexchange Involving Empty 4f Orbitals. Inorganic Chemistry, 2020, 59, 8716-8726.	4.0	12
56	Constructing a small strain potential for multi-scale modeling. Molecular Simulation, 2005, 31, 695-703.	2.0	11
57	Quantum, classical, and multi-scale simulation of silicaâ€“water interaction: molecules, clusters, and extended systems. Journal of Computer-Aided Materials Design, 2006, 13, 161-183.	0.7	11
58	Dynamics of Ag clusters on complex surfaces: Molecular dynamics simulations. Physical Review B, 2009, 79, .	3.2	11
59	Electronic Detection of Oxygen Adsorption and Sizeâ€Specific Doping of Fewâ€Atom Gold Clusters on Graphene. Advanced Materials Interfaces, 2018, 5, 1801274.	3.7	11
60	Three Jahn-Teller States of Matter in Spin-Crossover System Mn(taa). Physical Review Letters, 2020, 124, 227201.	7.8	11
61	Modified Surface Nanoscale Explosion:â€‰ Effects of Initial Condition and Charge Flow. Journal of Physical Chemistry B, 2000, 104, 4633-4641.	2.6	9
62	Resistance of Ag-silicene-Ag junctions: A combined nonequilibrium Green's function and Boltzmann transport study. Physical Review B, 2013, 88, .	3.2	9
63	First-principles study of multicontrol graphene doping using light-switching molecules. Physical Review B, 2014, 89, .	3.2	9
64	Insights into negative differential resistance in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> Esaki diodes: A first-principles perspective. Physical Review B, 2020, 102, .	3.2	9
65	Exploring the Magnetic Properties of the Largest Single-Molecule Magnets. Journal of Physical Chemistry Letters, 2020, 11, 3789-3795.	4.6	9
66	Barriers to predictive high-throughput screening for spin-crossover. Computational Materials Science, 2022, 206, 111161.	3.0	9
67	Using light-switching molecules to modulate charge mobility in a quantum dot array. Physical Review B, 2014, 89, .	3.2	8
68	Analysis of Exchange Interactions in Dimers of Mn₃ Single-Molecule Magnets, and Their Sensitivity to External Pressure. Journal of Physical Chemistry C, 2020, 124, 14768-14774.	3.1	8
69	First-principles study of magnetism and electric field effects in 2D systems. AVS Quantum Science, 2020, 2, .	4.9	7
70	Plane-wave transport method for low-symmetry lattices and its application. Physical Review B, 2012, 86, .	3.2	6
71	Magnetic phase transition induced by electrostatic gating in two-dimensional square metal-organic frameworks. Physical Review B, 2018, 97, .	3.2	6
72	Gate field effects on the topological insulator BiSbTeSe2 interface. Applied Physics Letters, 2020, 116, 031601.	3.3	5

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73	Annealingâ€Induced Changes in the Atomic Structure of Amorphous Silica, Germania, and Tantala Using Accelerated Molecular Dynamics. Physica Status Solidi (B): Basic Research, 2021, 258, 2000519.	1.5	5
74	Adiabatic Spin Pump through a Molecular Antiferromagnet Ce₃Mn₈^{III}. Journal of Physical Chemistry C, 2018, 122, 1422-1429.	3.1	4
75	Long-Range Magnetic Exchange Pathways in Complex Clusters from First Principles. Journal of Physical Chemistry C, 2021, 125, 11124-11131.	3.1	4
76	Multiple control of few-layer Janus MoSSe systems. Physical Review Materials, 2021, 5, .	2.4	4
77	Performance Enhancement of APW+lo Calculations by Simplest Separation of Concerns. Computation, 2022, 10, 43.	2.0	4
78	Cation Substitution Effect on a Molecular Analogue of Perovskite Manganites. Journal of Physical Chemistry C, 2017, 121, 10893-10898.	3.1	3
79	Tunneling field-effect junctions with WS2 barrier. Journal of Physics and Chemistry of Solids, 2019, 128, 343-350.	4.0	3
80	Analysis of two-level systems and mechanical loss in amorphous ZrO2-doped Ta2O5 by non-cage-breaking and cage-breaking transitions. Journal of Chemical Physics, 2021, 154, 174502.	3.0	3
81	Many-body localization from random magnetic anisotropy. Physical Review Research, 2019, 1, .	3.6	3
82	Electronic control of strong magnetic anisotropy in Co-based single-molecule magnets. Physical Review B, 2021, 104, .	3.2	3
83	Single-molecule magnet <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>Mn</mml:mi><mml:mn>12</mml:mn></mml:msub></mml:math> on GaAs-supported graphene: Gate field effects from first principles. Physical Review B, 2022, 105, .	3.2	3
84	Flexibility of the factorized form of the unitary coupled cluster Ansatz. Journal of Chemical Physics, 2022, 156, 044106.	3.0	3
85	Low-Depth Unitary Coupled Cluster Theory for Quantum Computation. Journal of Chemical Theory and Computation, 2022, 18, 2193-2198.	5.3	3
86	Using Hyperoptimized Tensor Networks and First-Principles Electronic Structure to Simulate the Experimental Properties of the Giant {Mn₈₄} Torus. Journal of Physical Chemistry Letters, 2022, 13, 2365-2370.	4.6	3
87	Multicontrol Over Grapheneâ€“Molecule Hetereojunctions. ACS Omega, 2017, 2, 5824-5830.	3.5	2
88	Comparative investigation of electronic transport across three-dimensional nanojunctions. Physical Review B, 2017, 95, .	3.2	2
89	Tuning spin transport across two-dimensional organometallic junctions. Physical Review B, 2018, 97, .	3.2	2
90	Feasibility of ground state spin switching in a molecular analogue of the mixed-metal oxides with the perovskite structure. Polyhedron, 2020, 176, 114275.	2.2	2

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91	First-principles study of an <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>S</mml:mi><mml:mo>=</mml:mo><mml:mn>1 quasi one-dimensional quantum molecular magnetic material. Physical Review B, 2021, 103, .	3.2	2
92	Self-consistent effective Hamiltonian theory for fermionic many-body systems. International Journal of Modern Physics B, 2021, 35, 2150019.	2.0	2
93	Ligand Optimization of Exchange Interaction in Co(II) Dimer Single Molecule Magnet by Machine Learning. Journal of Physical Chemistry A, 2022, 126, 529-535.	2.5	2
94	Clarâ€™s Goblet on Graphene: Field-Modulated Charge Transfer in a Hydrocarbon Heterostructure. Journal of Physical Chemistry C, 2022, 126, 5640-5648.	3.1	2
95	First-principles calculation of gate-tunable ferromagnetism in magic-angle twisted bilayer graphene under pressure. Journal of Physics Condensed Matter, 2022, 34, 385501.	1.8	2
96	Embedding atom-jellium model for metal surface. European Physical Journal D, 2007, 43, 247-250.	1.3	1
97	CONTROL OF CONDUCTANCE AND MAGNETORESISTANCE OF MOLECULAR JUNCTIONS. Spin, 2014, 04, 1440011.	1.3	1
98	Spin dependent resonant electron tunneling through planar graphene barriers. Carbon, 2019, 144, 362-369.	10.3	1
99	Anomalous frequency dependence of magneto-electric effect in doped DTN. Physica B: Condensed Matter, 2021, 608, 412875.	2.7	1
100	Modeling carrier mobility in graphene as a sensitive probe of molecular magnets. Physical Review B, 2021, 103, .	3.2	1
101	Solvothermal synthesis of [Cr7S8(en)8Cl2]Cl3Â·2H2O with magnetically frustrated [Cr7S8]5+ doubleâ€cubes. Chemistry - A European Journal, 2021, , .	3.3	1
102	First-principles study of bilayer polymeric manganese phthalocyanine. Physical Review B, 2022, 105, .	3.2	1