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	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
2	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
3	Flexibility of the factorized form of the unitary coupled cluster Ansatz. Journal of Chemical Physics, 2022, 156, 044106.	3.0	3
4	Barriers to predictive high-throughput screening for spin-crossover. Computational Materials Science, 2022, 206, 111161.	3.0	9
5	Low-Depth Unitary Coupled Cluster Theory for Quantum Computation. Journal of Chemical Theory and Computation, 2022, 18, 2193-2198.	5.3	3
6	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
7	Performance Enhancement of APW+lo Calculations by Simplest Separation of Concerns. Computation, 2022, 10, 43.	2.0	4
8	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
9	First-principles study of bilayer polymeric manganese phthalocyanine. Physical Review B, 2022, 105, .	3.2	1
10	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
11	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
12	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
13	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:mrow></mml:math> quasi one-dimensional quantum molecular magnetic material. Physical Review B, 2021, 103, .	3.2	1
14	Anomalous frequency dependence of magneto-electric effect in doped DTN. Physica B: Condensed Matter, 2021, 608, 412875.	2.7	1
15	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
16	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
17	Long-Range Magnetic Exchange Pathways in Complex Clusters from First Principles. Journal of Physical Chemistry C, 2021, 125, 11124-11131.	3.1	4
18	Modeling carrier mobility in graphene as a sensitive probe of molecular magnets. Physical Review B, 2021, 103, .	3.2	1

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19	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
20	Multiple control of few-layer Janus MoSSe systems. Physical Review Materials, 2021, 5, .	2.4	4
21	First-principles theory for Schottky barrier physics. Physical Review B, 2021, 104, .	3.2	14
22	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
23	Electronic control of strong magnetic anisotropy in Co-based single-molecule magnets. Physical Review B, 2021, 104, .	3.2	3
24	Self-consistent effective Hamiltonian theory for fermionic many-body systems. International Journal of Modern Physics B, 2021, 35, 2150019.	2.0	2
25	Solvothermal synthesis of [Cr7S8(en)8Cl2]Cl3Â·2H2O with magnetically frustrated [Cr7S8]5+ doubleâ€cubes. Chemistry - A European Journal, 2021, , .	3.3	1
26	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
27	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
28	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
29	Application of Quantum Computing to Biochemical Systems: A Look to the Future. Frontiers in Chemistry, 2020, 8, 587143.	3.6	28
30	Three Jahn-Teller States of Matter in Spin-Crossover System Mn(taa). Physical Review Letters, 2020, 124, 227201.	7.8	11
31	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
32	First-principles study of magnetism and electric field effects in 2D systems. AVS Quantum Science, 2020, 2, .	4.9	7
33	Theoretical prediction of magnetic exchange coupling constants from broken-symmetry coupled cluster calculations. Journal of Chemical Physics, 2020, 152, 234115.	3.0	17
34	Gate field effects on the topological insulator BiSbTeSe2 interface. Applied Physics Letters, 2020, 116, 031601.	3.3	5
35	Decoherence in Molecular Electron Spin Qubits: Insights from Quantum Many-Body Simulations. Journal of Physical Chemistry Letters, 2020, 11, 2074-2078.	4.6	32
36	Exploring the Magnetic Properties of the Largest Single-Molecule Magnets. Journal of Physical Chemistry Letters, 2020, 11, 3789-3795.	4.6	9

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37	<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</mml:mi> 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
38	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
39	Magnetoelectric behavior via a spin state transition. Nature Communications, 2019, 10, 4043.	12.8	29
40	Spin dependent resonant electron tunneling through planar graphene barriers. Carbon, 2019, 144, 362-369.	10.3	1
41	Tunneling field-effect junctions with WS2 barrier. Journal of Physics and Chemistry of Solids, 2019, 128, 343-350.	4.0	3
42	Many-body localization from random magnetic anisotropy. Physical Review Research, 2019, 1, .	3.6	3
43	Adiabatic Spin Pump through a Molecular Antiferromagnet Ce₃Mn₈^{III}. Journal of Physical Chemistry C, 2018, 122, 1422-1429.	3.1	4
44	Tuning spin transport across two-dimensional organometallic junctions. Physical Review B, 2018, 97, .	3.2	2
45	Magnetic phase transition induced by electrostatic gating in two-dimensional square metal-organic frameworks. Physical Review B, 2018, 97, .	3.2	6
46	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
47	Topological insulator-metal transition and molecular electronics device based on zigzag phagraphene nanoribbon. Journal of Applied Physics, 2018, 124, .	2.5	14
48	Cation Substitution Effect on a Molecular Analogue of Perovskite Manganites. Journal of Physical Chemistry C, 2017, 121, 10893-10898.	3.1	3
49	Origin of the second peak in the mechanical loss function of amorphous silica. Physical Review B, 2017, 95, .	3.2	13
50	Two-dimensional lateral GaN/SiC heterostructures: First-principles studies of electronic and magnetic properties. Physical Review B, 2017, 95, .	3.2	22
51	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
52	Multicontrol Over Grapheneâ€“Molecule Hetereojunctions. ACS Omega, 2017, 2, 5824-5830.	3.5	2
53	Comparative investigation of electronic transport across three-dimensional nanojunctions. Physical Review B, 2017, 95, .	3.2	2
54	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:m the Matsubara-time domain: Implementation and benchmarks of semiconductors and insulators. Physical Review B, 2016, 93, .	3.2	23

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55	Molecular dynamics modeling of mechanical loss in amorphous tantala and titania-doped tantala. Physical Review B, 2016, 93, .	3.2	33
56	First-principles studies of electric field effects on the electronic structure of trilayer graphene. Physical Review B, 2016, 94, .	3.2	20
57	Electron transport in graphene/graphene side-contact junction by plane-wave multiple-scattering method. Physical Review B, 2015, 91, .	3.2	12
58	First-principles simulations of a graphene-based field-effect transistor. Physical Review B, 2015, 91, .	3.2	15
59	First-principles study of multicontrol graphene doping using light-switching molecules. Physical Review B, 2014, 89, .	3.2	9
60	All-electron GW quasiparticle band structures of group 14 nitride compounds. Journal of Chemical Physics, 2014, 141, 044709.	3.0	17
61	CONTROL OF CONDUCTANCE AND MAGNETORESISTANCE OF MOLECULAR JUNCTIONS. Spin, 2014, 04, 1440011.	1.3	1
62	Doping effects of Se vacancies in monolayer FeSe. Physical Review B, 2014, 89, .	3.2	36
63	Using light-switching molecules to modulate charge mobility in a quantum dot array. Physical Review B, 2014, 89, .	3.2	8
64	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
65	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
66	Unified interatomic potential and energy barrier distributions for amorphous oxides. Journal of Chemical Physics, 2013, 139, 154506.	3.0	35
67	Resistance of Ag-silicene-Ag junctions: A combined nonequilibrium Green's function and Boltzmann transport study. Physical Review B, 2013, 88, .	3.2	9
68	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
69	Reversible Spin Polarization at Hybrid Organicâ€“Ferromagnetic Interfaces. Journal of Physical Chemistry Letters, 2013, 4, 3508-3512.	4.6	18
70	Giant Molecular Magnetocapacitance. Physical Review Letters, 2013, 110, 217205.	7.8	15
71	Plane-wave transport method for low-symmetry lattices and its application. Physical Review B, 2012, 86, .	3.2	6
72	Electronic and transport properties of azobenzene monolayer junctions as molecular switches. Physical Review B, 2012, 86, .	3.2	22

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73	OPAL: A multiscale multicenter simulation package based on MPIâ€2 protocol. International Journal of Quantum Chemistry, 2011, 111, 4020-4029.	2.0	13
74	Anisotropic quasiparticle lifetimes in Fe-based superconductors. Physical Review B, 2011, 83, .	3.2	37
75	Perfect spin-filtering and giant magnetoresistance with Fe-terminated graphene nanoribbon. Applied Physics Letters, 2011, 99, .	3.3	19
76	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:ms Physical Review B, 2010, 81, .	3.2	190
77	First-principles study of Fe/MgO based magnetic tunnel junctions with Mg interlayers. Physical Review B, 2010, 82, .	3.2	28
78	Transition metal adatom and dimer adsorbed on graphene: Induced magnetization and electronic structures. Physical Review B, 2010, 81, .	3.2	234
79	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
80	Insensitivity ofd-wave pairing to disorder in the high-temperature cuprate superconductors. Physical Review B, 2009, 79, .	3.2	18
81	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
82	Dynamics of Ag clusters on complex surfaces: Molecular dynamics simulations. Physical Review B, 2009, 79, .	3.2	11
83	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 Effective Hamiltonian fromab initiostudies. Physical Review B, 2008, 77, .	3.2	245
84	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
85	Effects of strain and defects on the electron conductance of metallic carbon nanotubes. Physical Review B, 2007, 75, .	3.2	36
86	Ab Initio Calculation of a Graphene-Ribbon-Based Molecular Switch. Journal of Physical Chemistry C, 2007, 111, 14266-14273.	3.1	27
87	Embedding atom-jellium model for metal surface. European Physical Journal D, 2007, 43, 247-250.	1.3	1
88	Current-voltage characteristics through a single light-sensitive molecule. Physical Review B, 2006, 73, .	3.2	87
89	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
90	First-principles investigation of a monolayer ofC60onhâ€™BNâ€•Ni(111). Physical Review B, 2005, 72, .	3.2	18

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91	Constructing a small strain potential for multi-scale modeling. Molecular Simulation, 2005, 31, 695-703.	2.0	11
92	Electronic structure and spin-dependent tunneling conductance under a finite bias. Physical Review B, 2004, 69, .	3.2	66
93	Coherent Electron Transport through an Azobenzene Molecule: A Light-Driven Molecular Switch. Physical Review Letters, 2004, 92, 158301.	7.8	249
94	Water-silica interaction in clusters. European Physical Journal D, 2003, 24, 323-326.	1.3	15
95	Transparent interface between classical molecular dynamics and first-principles molecular dynamics. International Journal of Quantum Chemistry, 2003, 93, 1-8.	2.0	16
96	Bulk Separative Enrichment in Metallic or Semiconducting Single-Walled Carbon Nanotubes. Nano Letters, 2003, 3, 1245-1249.	9.1	246
97	The stability of free and oxidized silver clusters. Journal of Chemical Physics, 2003, 118, 10956-10962.	3.0	44
98	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
99	Modified Surface Nanoscale Explosion:â€‰ Effects of Initial Condition and Charge Flow. Journal of Physical Chemistry B, 2000, 104, 4633-4641.	2.6	9
100	Cluster-surface collisions: Characteristics of Xe55- and C20â€“Si[111] surface bombardment. Journal of Chemical Physics, 1999, 111, 7583-7592.	3.0	17
101	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
102	A quantum molecular dynamics study of the properties of NO+(H2O)n clusters. Journal of Chemical Physics, 1998, 108, 2015-2023.	3.0	23