Haowei Peng

List of Publications by Citations

54 papers	3,374 citations	32 h-index	57 g-index
57 ext. papers	3,914 ext. citations	7.2 avg, IF	5.45 L-index

#	Paper	IF	Citations
54	Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional. *Nature Chemistry*, **2016**, 8, 831-6	17.6	480
53	Origin and enhancement of hole-induced ferromagnetism in first-row d0 semiconductors. *Physical Review Letters*, **2009**, 102, 017201	7.4	355
52	Understanding band gaps of solids in generalized Kohn-Sham theory. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 2801-2806	11.5	280
51	Versatile van der Waals Density Functional Based on a Meta-Generalized Gradient Approximation. *Physical Review X*, **2016**, 6,	9.1	213
50	Energetics of MnO2 polymorphs in density functional theory. *Physical Review B*, **2016**, 93,	3.3	147
49	More realistic band gaps from meta-generalized gradient approximations: Only in a generalized Kohn-Sham scheme. *Physical Review B*, **2016**, 93,	3.3	135
48	Possible origin of ferromagnetism in undoped anatase TiO2. *Physical Review B*, **2009**, 79,	3.3	127
47	Efficient first-principles prediction of solid stability: Towards chemical accuracy. *Npj Computational Materials*, **2018**, 4,	10.9	107
46	Evaluation of photovoltaic materials within the Cu-Sn-S family. *Applied Physics Letters*, **2013**, 103, 253902	3.4	106
45	A computational framework for automation of point defect calculations. *Computational Materials Science*, **2017**, 130, 1-9	3.2	83
44	Convergence of density and hybrid functional defect calculations for compound semiconductors. *Physical Review B*, **2013**, 88,	3.3	77
43	Semiconducting transition-metal oxides based on d5 cations: Theory for MnO and Fe2O3. *Physical Review B*, **2012**, 85,	3.3	66
42	Influence of ZnS and MgO Shell on the Photoluminescence Properties of ZnO Core/Shell Nanowires. *Journal of Physical Chemistry C*, **2010**, 114, 1467-1471	3.8	64
41	Giant Gating Tunability of Optical Refractive Index in Transition Metal Dichalcogenide Monolayers. *Nano Letters*, **2017**, 17, 3613-3618	11.5	59
40	Rehabilitation of the Perdew-Burke-Ernzerhof generalized gradient approximation for layered materials. *Physical Review B*, **2017**, 95,	3.3	58
39	Li-Doped Cr2MnO4: A New p-Type Transparent Conducting Oxide by Computational Materials Design. *Advanced Functional Materials*, **2013**, 23, 5267-5276	15.6	50
38	Electronic structure and transport properties of doped PbSe. *Physical Review B*, **2011**, 84,	3.3	50

37	First-principles study of native defects in rutile TiO2. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2008**, 372, 1527-1530	2.3	50
36	Effect of extended strain fields on point defect phonon scattering in thermoelectric materials. *Physical Chemistry Chemical Physics*, **2015**, 17, 19410-23	3.6	48
35	Band crossing in isovalent semiconductor alloys with large size mismatch: First-principles calculations of the electronic structure of Bi and N incorporated GaAs. *Physical Review B*, **2010**, 82,	3.3	48
34	Quantum Confinement and Electronic Properties of Rutile TiO2 Nanowires. *Journal of Physical Chemistry C*, **2008**, 112, 20241-20245	3.8	47
33	Polymorphic energy ordering of MgO, ZnO, GaN, and MnO within the random phase approximation. *Physical Review B*, **2013**, 87,	3.3	45
32	First-principles study of the electronic structures and magnetic properties of 3d transition metal-doped anatase TiO2. *Journal of Physics Condensed Matter*, **2008**, 20, 125207	1.8	45
31	First-Principles Study on Rutile TiO2 Quantum Dots. *Journal of Physical Chemistry C*, **2008**, 112, 13964-13969	3.8	41
30	Electronic Properties of Nonstoichiometric PbSe Quantum Dots from First Principles. *Journal of Physical Chemistry C*, **2009**, 113, 21506-21511	3.8	38
29	Novel phase diagram behavior and materials design in heterostructural semiconductor alloys. *Science Advances*, **2017**, 3, e1700270	14.3	37
28	Possible n□ype carrier sources in In2O3(ZnO)k. *Chemistry of Materials*, **2012**, 24, 106-114	9.6	37
27	Trade-Offs in Thin Film Solar Cells with Layered Chalcostibite Photovoltaic Absorbers. *Advanced Energy Materials*, **2017**, 7, 1601935	21.8	35
26	Systematic Doping of Cobalt into Layered Manganese Oxide Sheets Substantially Enhances Water Oxidation Catalysis. *Inorganic Chemistry*, **2018**, 57, 557-564	5.1	35
25	Using design principles to systematically plan the synthesis of hole-conducting transparent oxides: Cu3VO4 and Ag3VO4 as a case study. *Physical Review B*, **2011**, 84,	3.3	34
24	Electronic and thermoelectric analysis of phases in the In2O3(ZnO)k system. *Journal of Applied Physics*, **2011**, 109, 013713	2.5	34
23	Water Oxidation Catalyzed by Cobalt Oxide Supported on the Mattagamite Phase of CoTe2. *ACS Catalysis*, **2016**, 6, 7393-7397	13.1	32
22	Design of Semiconducting Tetrahedral Mn1□ZnxO Alloys and Their Application to Solar Water Splitting. *Physical Review X*, **2015**, 5,	9.1	30
21	Redox properties of birnessite from a defect perspective. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 9523-9528	11.5	30
20	Rethinking CO adsorption on transition-metal surfaces: Effect of density-driven self-interaction errors. *Physical Review B*, **2019**, 100,	3.3	29

19	Synergy of van der Waals and self-interaction corrections in transition metal monoxides. *Physical Review B*, **2017**, 96,	3.3	29
18	Characterization of defects in copper antimony disulfide. *Journal of Materials Chemistry A*, **2017**, 5, 21986-21993	9.6	23
17	Structural, Optical, and Transport Properties of □and □Ag3VO4. *Chemistry of Materials*, **2012**, 24, 3346-3354	9.6	23
16	Pathway to oxide photovoltaics via band-structure engineering of SnO. *APL Materials*, **2016**, 4, 106103	5.7	23
15	Synthesis and Characterization of (Sn,Zn)O Alloys. *Chemistry of Materials*, **2016**, 28, 7765-7772	9.6	15
14	Anisotropic Conductivity at the Single-Molecule Scale. *Angewandte Chemie - International Edition*, **2019**, 58, 14275-14280	16.4	14
13	Communication: Near-locality of exchange and correlation density functionals for 1- and 2-electron systems. *Journal of Chemical Physics*, **2016**, 144, 191101	3.9	14
12	Experimental Characterization of a Theoretically Designed Candidate p-Type Transparent Conducting Oxide: Li-Doped Cr2MnO4. *Chemistry of Materials*, **2014**, 26, 4598-4604	9.6	13
11	Potential-Induced High-Conductance Transport Pathways through Single-Molecule Junctions. *Journal of the American Chemical Society*, **2019**, 141, 10109-10116	16.4	11
10	Multivalency of Group 15 Dopants in SnO2. *Chemistry of Materials*, **2014**, 26, 4876-4881	9.6	11
9	Defect mechanisms in the In2O3(ZnO)k system (k = 3, 5, 7, 9). *Journal of Applied Physics*, **2012**, 112, 093712	2.5	11
8	Chemical trends of magnetic interaction in Mn-doped III-V semiconductors. *Applied Physics Letters*, **2013**, 102, 122409	3.4	10
7	Anisotropic Conductivity at the Single-Molecule Scale. *Angewandte Chemie*, **2019**, 131, 14413-14418	3.6	6
6	KAg11(VO4)4 as a candidate p-type transparent conducting oxide. *Journal of Chemical Physics*, **2013**, 138, 194703	3.9	6
5	High-Throughput Experimental Study of Wurtzite Mn Zn O Alloys for Water Splitting Applications. *ACS Omega*, **2019**, 4, 7436-7447	3.9	4
4	Different bonding type along each crystallographic axis: Computational study of poly(p-phenylene terephthalamide). *Physical Review Materials*, **2020**, 4,	3.2	3
3	Predictive design of intrinsic half-metallicity in zigzag tungsten dichalcogenide nanoribbons. *Physical Review B*, **2019**, 100,	3.3	3
2	Innentitelbild: Anisotropic Conductivity at the Single-Molecule Scale (Angew. Chem. 40/2019). *Angewandte Chemie*, **2019**, 131, 14138-14138	3.6	1

1	Reimagining the eg1 Electronic State in Oxygen Evolution Catalysis: Oxidation-State-Modulated Superlattices as a New Type of Heterostructure for Maximizing Catalysis. *Advanced Energy Materials*, **2021**, 11, 2101636	21.8	0