Patrick Rinke

List of Publications by Year in Descending Order

121 papers	7,916 citations	52 h-index	87 g-index
143 ext. papers	9,064 ext. citations	5.5 avg, IF	6.38 L-index

#	Paper	IF	Citations
121	All-Electron BSE@ Method for -Edge Core Electron Excitation Energies.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	1
120	Machine learning as a tool to engineer microstructures: Morphological prediction of tannin-based colloids using Bayesian surrogate models.. *MRS Bulletin*, **2022**, 47, 1-9	3.2	1
119	Improved One-Shot Total Energies from the Linearized GW Density Matrix. *Journal of Chemical Theory and Computation*, **2021**, 17, 2126-2136	6.4	3
118	Surface Functionalization of 2D MXenes: Trends in Distribution, Composition, and Electronic Properties. *Journal of Physical Chemistry Letters*, **2021**, 12, 2377-2384	6.4	23
117	Real-time time-dependent density functional theory implementation of electronic circular dichroism applied to nanoscale metal-organic clusters. *Journal of Chemical Physics*, **2021**, 154, 114102	3.9	6
116	Integrating Bayesian Inference with Scanning Probe Experiments for Robust Identification of Surface Adsorbate Configurations. *Advanced Functional Materials*, **2021**, 31, 2010853	15.6	1
115	Electronic Characterization of a Charge-Transfer Complex Monolayer on Graphene. *ACS Nano*, **2021** , 15, 9945-9954	16.7	2
114	Efficient Amino Acid Conformer Search with Bayesian Optimization. *Journal of Chemical Theory and Computation*, **2021**, 17, 1955-1966	6.4	9
113	Atomic and electronic structure of cesium lead triiodide surfaces. *Journal of Chemical Physics*, **2021**, 154, 074712	3.9	1
112	Assessing the Approach: Beyond with Hedin's Full Second-Order Self-Energy Contribution. *Journal of Chemical Theory and Computation*, **2021**, 17, 5140-5154	6.4	3
111	Integrating Bayesian Inference with Scanning Probe Experiments for Robust Identification of Surface Adsorbate Configurations (Adv. Funct. Mater. 32/2021). *Advanced Functional Materials*, **2021**, 31, 2170235	15.6	
110	Charge Transfer into Organic Thin Films: A Deeper Insight through Machine-Learning-Assisted Structure Search. *Advanced Science*, **2020**, 7, 2000992	13.6	17
109	Atomic structures and orbital energies of 61,489 crystal-forming organic molecules. *Scientific Data*, **2020**, 7, 58	8.2	23
108	Accurate Absolute and Relative Core-Level Binding Energies from. *Journal of Physical Chemistry Letters*, **2020**, 11, 1840-1847	6.4	31
107	Detecting stable adsorbates of (1)-camphor on Cu(111) with Bayesian optimization. *Beilstein Journal of Nanotechnology*, **2020**, 11, 1577-1589	3	7
106	Relativistic correction scheme for core-level binding energies from GW. *Journal of Chemical Physics*, **2020**, 153, 114110	3.9	10
105	DScribe: Library of descriptors for machine learning in materials science. *Computer Physics Communications*, **2020**, 247, 106949	4.2	178

104	Database-driven high-throughput study of coating materials for hybrid perovskites. *New Journal of Physics*, **2019**, 21, 083018	2.9	4
103	Deep Learning Spectroscopy: Neural Networks for Molecular Excitation Spectra. *Advanced Science*, **2019**, 6, 1801367	13.6	100
102	The Compendium: A Practical Guide to Theoretical Photoemission Spectroscopy. *Frontiers in Chemistry*, **2019**, 7, 377	5	139
101	Chemical diversity in molecular orbital energy predictions with kernel ridge regression. *Journal of Chemical Physics*, **2019**, 150, 204121	3.9	27
100	Machine Learning: Deep Learning Spectroscopy: Neural Networks for Molecular Excitation Spectra (Adv. Sci. 9/2019). *Advanced Science*, **2019**, 6, 1970053	13.6	5
99	Dynamical configuration interaction: Quantum embedding that combines wave functions and Green's functions. *Physical Review B*, **2019**, 99,	3.3	12
98	Bayesian inference of atomistic structure in functional materials. *Npj Computational Materials*, **2019** , 5,	10.9	50
97	Data-Driven Materials Science: Status, Challenges, and Perspectives. *Advanced Science*, **2019**, 6, 1900808	13.6	162
96	Gold diggers: Altered reconstruction of the gold surface by physisorbed aromatic oligomers. *Physical Review Materials*, **2019**, 3,	3.2	3
95	Quantum embedding theory in the screened Coulomb interaction: Combining configuration interaction with GW/BSE. *Physical Review Materials*, **2019**, 3,	3.2	7
94	Formation of graphene atop a Si adlayer on the C-face of SiC. *Physical Review Materials*, **2019**, 3,	3.2	3
93	Electron-phonon coupling in d-electron solids: A temperature-dependent study of rutile TiO2 by first-principles theory and two-photon photoemission. *Physical Review Research*, **2019**, 1,	3.9	5
92	First-principles supercell calculations of small polarons with proper account for long-range polarization effects. *New Journal of Physics*, **2018**, 20, 033023	2.9	25
91	Theory of Excitation Transfer between Two-Dimensional Semiconductor and Molecular Layers. *Physical Review Applied*, **2018**, 9,	4.3	2
90	Activation Energy of Organic Cation Rotation in CHNHPbI and CDNHPbI: Quasi-Elastic Neutron Scattering Measurements and First-Principles Analysis Including Nuclear Quantum Effects. *Journal of Physical Chemistry Letters*, **2018**, 9, 3969-3977	6.4	26
89	Machine learning hydrogen adsorption on nanoclusters through structural descriptors. *Npj Computational Materials*, **2018**, 4,	10.9	93
88	Multiscale model for disordered hybrid perovskites: The concept of organic cation pair modes. *Physical Review B*, **2018**, 98,	3.3	12
87	Optical Properties of Silver-Mediated DNA from Molecular Dynamics and Time Dependent Density Functional Theory. *International Journal of Molecular Sciences*, **2018**, 19,	6.3	5

86	Core-Level Binding Energies from GW: An Efficient Full-Frequency Approach within a Localized Basis. *Journal of Chemical Theory and Computation*, **2018**, 14, 4856-4869	6.4	55
85	Multi-scale model for the structure of hybrid perovskites: analysis of charge migration in disordered MAPbI3 structures. *New Journal of Physics*, **2018**, 20, 103013	2.9	3
84	Materials structure genealogy and high-throughput topological classification of surfaces and 2D materials. *Npj Computational Materials*, **2018**, 4,	10.9	6
83	All-electron, real-space perturbation theory for homogeneous electric fields: theory, implementation, and application within DFT. *New Journal of Physics*, **2018**, 20, 073040	2.9	20
82	Global and local aspects of the surface potential landscape for energy level alignment at organic-ZnO interfaces. *Chemical Physics*, **2017**, 485-486, 149-165	2.3	16
81	Band Bending Engineering at Organic/Inorganic Interfaces Using Organic Self-Assembled Monolayers. *Advanced Electronic Materials*, **2017**, 3, 1600373	6.4	13
80	Lattice dynamics calculations based on density-functional perturbation theory in real space. *Computer Physics Communications*, **2017**, 215, 26-46	4.2	27
79	On the Monte Carlo Description of Hot Carrier Effects and Device Characteristics of III-N LEDs. *Advanced Electronic Materials*, **2017**, 3, 1600494	6.4	13
78	Charge-Transfer-Driven Nonplanar Adsorption of FTCNQ Molecules on Epitaxial Graphene. *ACS Nano*, **2017**, 11, 4960-4968	16.7	41
77	Doping dependence of the surface phase stability of polar O-terminated (0001) ZnO. *New Journal of Physics*, **2017**, 19, 083012	2.9	10
76	Benchmark of GW Approaches for the GW100 Test Set. *Journal of Chemical Theory and Computation* , **2016**, 12, 5076-5087	6.4	63
75	Towards Efficient Orbital-Dependent Density Functionals for Weak and Strong Correlation. *Physical Review Letters*, **2016**, 117, 133002	7.4	18
74	Density functional theory study of the δ-γ phase transition in cerium: Role of electron correlation and f-orbital localization. *Physical Review B*, **2016**, 93,	3.3	15
73	Piecewise linearity in the GW approximation for accurate quasiparticle energy predictions. *Physical Review B*, **2016**, 93,	3.3	21
72	Atomic structure of metal-halide perovskites from first principles: The chicken-and-egg paradox of the organic-inorganic interaction. *Physical Review B*, **2016**, 94,	3.3	53
71	Enforcing the linear behavior of the total energy with hybrid functionals: Implications for charge transfer, interaction energies, and the random-phase approximation. *Physical Review B*, **2016**, 94,	3.3	40
70	Self-consistent Green's function embedding for advanced electronic structure methods based on a dynamical mean-field concept. *Physical Review B*, **2016**, 93,	3.3	26
69	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules II: Non-Empirically Tuned Long-Range Corrected Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2016**, 12, 605-14	6.4	62

68	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules III: A Benchmark of GW Methods. *Journal of Chemical Theory and Computation*, **2016**, 12, 615-26	6.4	119
67	Wave-function inspired density functional applied to the H2/${{rm{H}}}_{2}^{+}$ challenge. *New Journal of Physics*, **2016**, 18, 073026	2.9	10
66	Hybrid functionals for large periodic systems in an all-electron, numeric atom-centered basis framework. *Computer Physics Communications*, **2015**, 192, 60-69	4.2	89
65	Multiscale approach to the electronic structure of doped semiconductor surfaces. *Physical Review B* , **2015**, 91,	3.3	24
64	Evidence for photogenerated intermediate hole polarons in ZnO. *Nature Communications*, **2015**, 6, 6901	17.4	42
63	GW100: Benchmarking G0W0 for Molecular Systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 5665-87	6.4	207
62	Accurate localized resolution of identity approach for linear-scaling hybrid density functionals and for many-body perturbation theory. *New Journal of Physics*, **2015**, 17, 093020	2.9	65
61	Why graphene growth is very different on the C face than on the Si face of SiC: Insights from surface equilibria and the (3□)□C□SiC(1□1□1□) reconstruction. *Physical Review B*, **2015**, 91,	3.3	11
60	First-principles calculations of indirect Auger recombination in nitride semiconductors. *Physical Review B*, **2015**, 92,	3.3	57
59	Beyond the GW approximation: A second-order screened exchange correction. *Physical Review B*, **2015**, 92,	3.3	37
58	Static correlation and electron localization in molecular dimers from the self-consistent RPA and GW approximation. *Physical Review B*, **2015**, 91,	3.3	46
57	Length dependence of ionization potentials of transacetylenes: Internally consistent DFT/GW approach. *Physical Review B*, **2015**, 92,	3.3	25
56	Integer versus Fractional Charge Transfer at Metal(/Insulator)/Organic Interfaces: Cu(/NaCl)/TCNE. *ACS Nano*, **2015**, 9, 5391-404	16.7	48
55	Influence of hydrogen on the structure and stability of ultra-thin ZnO on metal substrates. *Applied Physics Letters*, **2015**, 106, 131602	3.4	11
54	First-principles description of charge transfer in donor-acceptor compounds from self-consistent many-body perturbation theory. *Physical Review B*, **2014**, 90,	3.3	42
53	Effects of strain on the band structure of group-III nitrides. *Physical Review B*, **2014**, 90,	3.3	73
52	Theory of optical excitations in dipole-coupled hybrid molecule-semiconductor layers: Coupling of a molecular resonance to semiconductor continuum states. *Physical Review B*, **2014**, 89,	3.3	7
51	Thermodynamic equilibrium conditions of graphene films on SiC. *Physical Review Letters*, **2013**, 111, 065502	7.4	32

50	Self-consistent GW: All-electron implementation with localized basis functions. *Physical Review B*, **2013**, 88,	3.3	120
49	Raman study of 2,7-bis(biphenyl-4-yl-)2?,7?-ditertbutyl-9,9?-spirobifluorene adsorbed on oxide surfaces. *Chemical Physics Letters*, **2013**, 584, 74-78	2.5	3
48	Enhanced Optical Absorption Due to Symmetry Breaking in TiO2(1⊠)S2x Alloys. *Journal of Physical Chemistry C*, **2013**, 117, 4189-4193	3.8	13
47	Bond breaking and bond formation: how electron correlation is captured in many-body perturbation theory and density-functional theory. *Physical Review Letters*, **2013**, 110, 146403	7.4	69
46	Controlling the work function of ZnO and the energy-level alignment at the interface to organic semiconductors with a molecular electron acceptor. *Physical Review B*, **2013**, 87,	3.3	96
45	Space-charge transfer in hybrid inorganic-organic systems. *Physical Review Letters*, **2013**, 111, 226802	7.4	59
44	Hybrid density functional theory meets quasiparticle calculations: A consistent electronic structure approach. *Physical Review B*, **2013**, 88,	3.3	99
43	Stabilization of semiconductor surfaces through bulk dopants. *New Journal of Physics*, **2013**, 15, 083009	2.9	22
42	Interface dipoles of organic molecules on Ag(111) in hybrid density-functional theory. *New Journal of Physics*, **2013**, 15, 123028	2.9	54
41	Large work function reduction by adsorption of a molecule with a negative electron affinity: pyridine on ZnO(1010). *Journal of Chemical Physics*, **2013**, 139, 174701	3.9	62
40	Numeric atom-centered-orbital basis sets with valence-correlation consistency from H to Ar. *New Journal of Physics*, **2013**, 15, 123033	2.9	65
39	Renormalized second-order perturbation theory for the electron correlation energy: Concept, implementation, and benchmarks. *Physical Review B*, **2013**, 88,	3.3	88
38	Random-phase approximation and its applications in computational chemistry and materials science. *Journal of Materials Science*, **2012**, 47, 7447-7471	4.3	389
37	Strain effects and band parameters in MgO, ZnO, and CdO. *Applied Physics Letters*, **2012**, 101, 152105	3.4	56
36	Electronic properties of lanthanide oxides from the GW perspective. *Physical Review B*, **2012**, 86,	3.3	86
35	New perspective on formation energies and energy levels of point defects in nonmetals. *Physical Review Letters*, **2012**, 108, 066404	7.4	93
34	Benchmark of GW methods for azabenzenes. *Physical Review B*, **2012**, 86,	3.3	132
33	First-principles optical spectra for F centers in MgO. *Physical Review Letters*, **2012**, 108, 126404	7.4	131

32	Resolution-of-identity approach to Hartree□Fock, hybrid density functionals, RPA, MP2 andGWwith numeric atom-centered orbital basis functions. *New Journal of Physics*, **2012**, 14, 053020	2.9	411
31	Assessment of correlation energies based on the random-phase approximation. *New Journal of Physics*, **2012**, 14, 043002	2.9	111
30	Density-functional theory for f-electron systems: the □phase transition in cerium. *Physical Review Letters*, **2012**, 109, 146402	7.4	51
29	Beyond the random-phase approximation for the electron correlation energy: the importance of single excitations. *Physical Review Letters*, **2011**, 106, 153003	7.4	171
28	Indirect Auger recombination as a cause of efficiency droop in nitride light-emitting diodes. *Applied Physics Letters*, **2011**, 98, 161107	3.4	388
27	Band parameters and strain effects in ZnO and group-III nitrides. *Semiconductor Science and Technology*, **2011**, 26, 014037	1.8	48
26	Role of strain in polarization switching in semipolar InGaN/GaN quantum wells. *Applied Physics Letters*, **2010**, 97, 181102	3.4	29
25	First-principles modeling of localized d states with the GW@LDA+U approach. *Physical Review B*, **2010**, 82,	3.3	188
24	Free-carrier absorption in nitrides from first principles. *Physical Review B*, **2010**, 81,	3.3	97
23	Large-scale surface reconstruction energetics of Pt(100) and Au(100) by all-electron density functional theory. *Physical Review B*, **2010**, 82,	3.3	46
22	Determination of Internal Loss in Nitride Lasers from First Principles. *Applied Physics Express*, **2010**, 3, 082101	2.4	56
21	Electronic band structure of zirconia and hafnia polymorphs from the GW perspective. *Physical Review B*, **2010**, 81,	3.3	157
20	Exploring the random phase approximation: Application to CO adsorbed on Cu(111). *Physical Review B*, **2009**, 80,	3.3	136
19	Controlling polarization at insulating surfaces: quasiparticle calculations for molecules adsorbed on insulator films. *Physical Review Letters*, **2009**, 103, 056803	7.4	62
18	Auger recombination rates in nitrides from first principles. *Applied Physics Letters*, **2009**, 94, 191109	3.4	297
17	Defect formation energies without the band-gap problem: combining density-functional theory and the GW approach for the silicon self-interstitial. *Physical Review Letters*, **2009**, 102, 026402	7.4	196
16	Strain effects in group-III nitrides: Deformation potentials for AlN, GaN, and InN. *Applied Physics Letters*, **2009**, 95, 121111	3.4	132
15	Localized and itinerant states in lanthanide oxides united by GW @ LDA+U. *Physical Review Letters*, **2009**, 102, 126403	7.4	142

14	Screening in two dimensions: GW calculations for surfaces and thin films using the repeated-slab approach. *Physical Review B*, **2008**, 77,	3.3	56
13	Consistent set of band parameters for the group-III nitrides AlN, GaN, and InN. *Physical Review B*, **2008**, 77,	3.3	306
12	Optimizing optical absorption of TiO2 by alloying with TiS2. *Applied Physics Letters*, **2008**, 92, 041104	3.4	20
11	Exciting prospects for solids: Exact-exchange based functionals meet quasiparticle energy calculations. *Physica Status Solidi (B): Basic Research*, **2008**, 245, 929-945	1.3	82
10	Dielectric anisotropy in the GW space-time method. *Computer Physics Communications*, **2007**, 176, 1-13	4.2	43
9	Ultrathin oxides: bulk-oxide-like model surfaces or unique films?. *Physical Review Letters*, **2007**, 99, 086101	7.4	52
8	Self-interaction in Green-function theory of the hydrogen atom. *Physical Review A*, **2007**, 75,	2.6	54
7	Vertex corrections in localized and extended systems. *Physical Review B*, **2007**, 76,	3.3	40
6	Exact-exchange-based quasiparticle energy calculations for the band gap, effective masses, and deformation potentials of ScN. *Physical Review B*, **2006**, 74,	3.3	78
5	CombiningGWcalculations with exact-exchange density-functional theory: an analysis of valence-band photoemission for compound semiconductors. *New Journal of Physics*, **2005**, 7, 126-126	2.9	250
4	Image states in metal clusters. *Physical Review A*, **2004**, 70,	2.6	32
3	Comment on "band-gap problem in semiconductors revisited: effects of core States and many-body self-consistency". *Physical Review Letters*, **2004**, 93, 249701; author reply 249702	7.4	59
2	Image resonance in the many-body density of states at a metal surface. *Physical Review B*, **2003**, 68,	3.3	23
1	Lithium-Ion Battery Technology for Voltage Control of Perpendicular Magnetization. *Advanced Functional Materials*,2113118	15.6	2