

# Patrick Rinke

## List of Publications by Citations

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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	Resolution-of-identity approach to Hartree-Fock, hybrid density functionals, RPA, MP2 and GW with numeric atom-centered orbital basis functions. <i>New Journal of Physics</i> , <b>2012</b> , 14, 053020	2.9	411
120	Random-phase approximation and its applications in computational chemistry and materials science. <i>Journal of Materials Science</i> , <b>2012</b> , 47, 7447-7471	4.3	389
119	Indirect Auger recombination as a cause of efficiency droop in nitride light-emitting diodes. <i>Applied Physics Letters</i> , <b>2011</b> , 98, 161107	3.4	388
118	Consistent set of band parameters for the group-III nitrides AlN, GaN, and InN. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	306
117	Auger recombination rates in nitrides from first principles. <i>Applied Physics Letters</i> , <b>2009</b> , 94, 191109	3.4	297
116	Combining GW calculations with exact-exchange density-functional theory: an analysis of valence-band photoemission for compound semiconductors. <i>New Journal of Physics</i> , <b>2005</b> , 7, 126-126	2.9	250
115	GW100: Benchmarking G0W0 for Molecular Systems. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 5665-87	6.4	207
114	Defect formation energies without the band-gap problem: combining density-functional theory and the GW approach for the silicon self-interstitial. <i>Physical Review Letters</i> , <b>2009</b> , 102, 026402	7.4	196
113	First-principles modeling of localized d states with the GW@LDA+U approach. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	188
112	Dscribe: Library of descriptors for machine learning in materials science. <i>Computer Physics Communications</i> , <b>2020</b> , 247, 106949	4.2	178
111	Beyond the random-phase approximation for the electron correlation energy: the importance of single excitations. <i>Physical Review Letters</i> , <b>2011</b> , 106, 153003	7.4	171
110	Data-Driven Materials Science: Status, Challenges, and Perspectives. <i>Advanced Science</i> , <b>2019</b> , 6, 1900808	13.6	162
109	Electronic band structure of zirconia and hafnia polymorphs from the GW perspective. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	157
108	Localized and itinerant states in lanthanide oxides united by GW @ LDA+U. <i>Physical Review Letters</i> , <b>2009</b> , 102, 126403	7.4	142
107	The Compendium: A Practical Guide to Theoretical Photoemission Spectroscopy. <i>Frontiers in Chemistry</i> , <b>2019</b> , 7, 377	5	139
106	Exploring the random phase approximation: Application to CO adsorbed on Cu(111). <i>Physical Review B</i> , <b>2009</b> , 80,	3.3	136
105	Benchmark of GW methods for azabenzenes. <i>Physical Review B</i> , <b>2012</b> , 86,	3.3	132

104	Strain effects in group-III nitrides: Deformation potentials for AlN, GaN, and InN. <i>Applied Physics Letters</i> , <b>2009</b> , 95, 121111	3.4	132
103	First-principles optical spectra for F centers in MgO. <i>Physical Review Letters</i> , <b>2012</b> , 108, 126404	7.4	131
102	Self-consistent GW: All-electron implementation with localized basis functions. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	120
101	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules III: A Benchmark of GW Methods. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 615-26	6.4	119
100	Assessment of correlation energies based on the random-phase approximation. <i>New Journal of Physics</i> , <b>2012</b> , 14, 043002	2.9	111
99	Deep Learning Spectroscopy: Neural Networks for Molecular Excitation Spectra. <i>Advanced Science</i> , <b>2019</b> , 6, 1801367	13.6	100
98	Hybrid density functional theory meets quasiparticle calculations: A consistent electronic structure approach. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	99
97	Free-carrier absorption in nitrides from first principles. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	97
96	Controlling the work function of ZnO and the energy-level alignment at the interface to organic semiconductors with a molecular electron acceptor. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	96
95	Machine learning hydrogen adsorption on nanoclusters through structural descriptors. <i>Npj Computational Materials</i> , <b>2018</b> , 4,	10.9	93
94	New perspective on formation energies and energy levels of point defects in nonmetals. <i>Physical Review Letters</i> , <b>2012</b> , 108, 066404	7.4	93
93	Hybrid functionals for large periodic systems in an all-electron, numeric atom-centered basis framework. <i>Computer Physics Communications</i> , <b>2015</b> , 192, 60-69	4.2	89
92	Renormalized second-order perturbation theory for the electron correlation energy: Concept, implementation, and benchmarks. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	88
91	Electronic properties of lanthanide oxides from the GW perspective. <i>Physical Review B</i> , <b>2012</b> , 86,	3.3	86
90	Exciting prospects for solids: Exact-exchange based functionals meet quasiparticle energy calculations. <i>Physica Status Solidi (B): Basic Research</i> , <b>2008</b> , 245, 929-945	1.3	82
89	Exact-exchange-based quasiparticle energy calculations for the band gap, effective masses, and deformation potentials of ScN. <i>Physical Review B</i> , <b>2006</b> , 74,	3.3	78
88	Effects of strain on the band structure of group-III nitrides. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	73
87	Bond breaking and bond formation: how electron correlation is captured in many-body perturbation theory and density-functional theory. <i>Physical Review Letters</i> , <b>2013</b> , 110, 146403	7.4	69

86	Accurate localized resolution of identity approach for linear-scaling hybrid density functionals and for many-body perturbation theory. <i>New Journal of Physics</i> , <b>2015</b> , 17, 093020	2.9	65
85	Numeric atom-centered-orbital basis sets with valence-correlation consistency from H to Ar. <i>New Journal of Physics</i> , <b>2013</b> , 15, 123033	2.9	65
84	Benchmark of GW Approaches for the GW100 Test Set. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 5076-5087	6.4	63
83	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules II: Non-Empirically Tuned Long-Range Corrected Hybrid Functionals. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 605-14	6.4	62
82	Large work function reduction by adsorption of a molecule with a negative electron affinity: pyridine on ZnO(1010). <i>Journal of Chemical Physics</i> , <b>2013</b> , 139, 174701	3.9	62
81	Controlling polarization at insulating surfaces: quasiparticle calculations for molecules adsorbed on insulator films. <i>Physical Review Letters</i> , <b>2009</b> , 103, 056803	7.4	62
80	Space-charge transfer in hybrid inorganic-organic systems. <i>Physical Review Letters</i> , <b>2013</b> , 111, 226802	7.4	59
79	Comment on "band-gap problem in semiconductors revisited: effects of core States and many-body self-consistency". <i>Physical Review Letters</i> , <b>2004</b> , 93, 249701; author reply 249702	7.4	59
78	First-principles calculations of indirect Auger recombination in nitride semiconductors. <i>Physical Review B</i> , <b>2015</b> , 92,	3.3	57
77	Strain effects and band parameters in MgO, ZnO, and CdO. <i>Applied Physics Letters</i> , <b>2012</b> , 101, 152105	3.4	56
76	Determination of Internal Loss in Nitride Lasers from First Principles. <i>Applied Physics Express</i> , <b>2010</b> , 3, 082101	2.4	56
75	Screening in two dimensions: GW calculations for surfaces and thin films using the repeated-slab approach. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	56
74	Core-Level Binding Energies from GW: An Efficient Full-Frequency Approach within a Localized Basis. <i>Journal of Chemical Theory and Computation</i> , <b>2018</b> , 14, 4856-4869	6.4	55
73	Interface dipoles of organic molecules on Ag(111) in hybrid density-functional theory. <i>New Journal of Physics</i> , <b>2013</b> , 15, 123028	2.9	54
72	Self-interaction in Green's-function theory of the hydrogen atom. <i>Physical Review A</i> , <b>2007</b> , 75,	2.6	54
71	Atomic structure of metal-halide perovskites from first principles: The chicken-and-egg paradox of the organic-inorganic interaction. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	53
70	Ultrathin oxides: bulk-oxide-like model surfaces or unique films?. <i>Physical Review Letters</i> , <b>2007</b> , 99, 086101	7.4	52
69	Density-functional theory for f-electron systems: the $\alpha$ -phase transition in cerium. <i>Physical Review Letters</i> , <b>2012</b> , 109, 146402	7.4	51

68	Bayesian inference of atomistic structure in functional materials. <i>Npj Computational Materials</i> , <b>2019</b> , 5,	10.9	50
67	Integer versus Fractional Charge Transfer at Metal(/Insulator)/Organic Interfaces: Cu(/NaCl)/TCNE. <i>ACS Nano</i> , <b>2015</b> , 9, 5391-404	16.7	48
66	Band parameters and strain effects in ZnO and group-III nitrides. <i>Semiconductor Science and Technology</i> , <b>2011</b> , 26, 014037	1.8	48
65	Static correlation and electron localization in molecular dimers from the self-consistent RPA and GW approximation. <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	46
64	Large-scale surface reconstruction energetics of Pt(100) and Au(100) by all-electron density functional theory. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	46
63	Dielectric anisotropy in the GW space-time method. <i>Computer Physics Communications</i> , <b>2007</b> , 176, 1-13	4.2	43
62	Evidence for photogenerated intermediate hole polarons in ZnO. <i>Nature Communications</i> , <b>2015</b> , 6, 6901	17.4	42
61	First-principles description of charge transfer in donor-acceptor compounds from self-consistent many-body perturbation theory. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	42
60	Charge-Transfer-Driven Nonplanar Adsorption of FTCNQ Molecules on Epitaxial Graphene. <i>ACS Nano</i> , <b>2017</b> , 11, 4960-4968	16.7	41
59	Enforcing the linear behavior of the total energy with hybrid functionals: Implications for charge transfer, interaction energies, and the random-phase approximation. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	40
58	Vertex corrections in localized and extended systems. <i>Physical Review B</i> , <b>2007</b> , 76,	3.3	40
57	Beyond the GW approximation: A second-order screened exchange correction. <i>Physical Review B</i> , <b>2015</b> , 92,	3.3	37
56	Thermodynamic equilibrium conditions of graphene films on SiC. <i>Physical Review Letters</i> , <b>2013</b> , 111, 065502	5.0	32
55	Image states in metal clusters. <i>Physical Review A</i> , <b>2004</b> , 70,	2.6	32
54	Accurate Absolute and Relative Core-Level Binding Energies from. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 1840-1847	6.4	31
53	Role of strain in polarization switching in semipolar InGaN/GaN quantum wells. <i>Applied Physics Letters</i> , <b>2010</b> , 97, 181102	3.4	29
52	Lattice dynamics calculations based on density-functional perturbation theory in real space. <i>Computer Physics Communications</i> , <b>2017</b> , 215, 26-46	4.2	27
51	Chemical diversity in molecular orbital energy predictions with kernel ridge regression. <i>Journal of Chemical Physics</i> , <b>2019</b> , 150, 204121	3.9	27

50	Self-consistent Green's function embedding for advanced electronic structure methods based on a dynamical mean-field concept. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	26
49	Activation Energy of Organic Cation Rotation in CHNHPbI and CDNHPbI: Quasi-Elastic Neutron Scattering Measurements and First-Principles Analysis Including Nuclear Quantum Effects. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 3969-3977	6.4	26
48	First-principles supercell calculations of small polarons with proper account for long-range polarization effects. <i>New Journal of Physics</i> , <b>2018</b> , 20, 033023	2.9	25
47	Length dependence of ionization potentials of transacetylenes: Internally consistent DFT/GW approach. <i>Physical Review B</i> , <b>2015</b> , 92,	3.3	25
46	Multiscale approach to the electronic structure of doped semiconductor surfaces. <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	24
45	Atomic structures and orbital energies of 61,489 crystal-forming organic molecules. <i>Scientific Data</i> , <b>2020</b> , 7, 58	8.2	23
44	Image resonance in the many-body density of states at a metal surface. <i>Physical Review B</i> , <b>2003</b> , 68,	3.3	23
43	Surface Functionalization of 2D MXenes: Trends in Distribution, Composition, and Electronic Properties. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 2377-2384	6.4	23
42	Stabilization of semiconductor surfaces through bulk dopants. <i>New Journal of Physics</i> , <b>2013</b> , 15, 083009	2.9	22
41	Piecewise linearity in the GW approximation for accurate quasiparticle energy predictions. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	21
40	Optimizing optical absorption of TiO <sub>2</sub> by alloying with TiS <sub>2</sub> . <i>Applied Physics Letters</i> , <b>2008</b> , 92, 041104	3.4	20
39	All-electron, real-space perturbation theory for homogeneous electric fields: theory, implementation, and application within DFT. <i>New Journal of Physics</i> , <b>2018</b> , 20, 073040	2.9	20
38	Towards Efficient Orbital-Dependent Density Functionals for Weak and Strong Correlation. <i>Physical Review Letters</i> , <b>2016</b> , 117, 133002	7.4	18
37	Charge Transfer into Organic Thin Films: A Deeper Insight through Machine-Learning-Assisted Structure Search. <i>Advanced Science</i> , <b>2020</b> , 7, 2000992	13.6	17
36	Global and local aspects of the surface potential landscape for energy level alignment at organic-ZnO interfaces. <i>Chemical Physics</i> , <b>2017</b> , 485-486, 149-165	2.3	16
35	Density functional theory study of the $\beta$ phase transition in cerium: Role of electron correlation and f-orbital localization. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	15
34	Band Bending Engineering at Organic/Inorganic Interfaces Using Organic Self-Assembled Monolayers. <i>Advanced Electronic Materials</i> , <b>2017</b> , 3, 1600373	6.4	13
33	On the Monte Carlo Description of Hot Carrier Effects and Device Characteristics of III-N LEDs. <i>Advanced Electronic Materials</i> , <b>2017</b> , 3, 1600494	6.4	13

32	Enhanced Optical Absorption Due to Symmetry Breaking in TiO <sub>2</sub> (1-x)S <sub>2x</sub> Alloys. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 4189-4193	3.8	13
31	Dynamical configuration interaction: Quantum embedding that combines wave functions and Green's functions. <i>Physical Review B</i> , <b>2019</b> , 99,	3.3	12
30	Multiscale model for disordered hybrid perovskites: The concept of organic cation pair modes. <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	12
29	Why graphene growth is very different on the C face than on the Si face of SiC: Insights from surface equilibria and the (3x3)R120° reconstruction. <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	11
28	Influence of hydrogen on the structure and stability of ultra-thin ZnO on metal substrates. <i>Applied Physics Letters</i> , <b>2015</b> , 106, 131602	3.4	11
27	Doping dependence of the surface phase stability of polar O-terminated (0001) ZnO. <i>New Journal of Physics</i> , <b>2017</b> , 19, 083012	2.9	10
26	Relativistic correction scheme for core-level binding energies from GW. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 114110	3.9	10
25	Wave-function inspired density functional applied to the H <sub>2</sub> /H <sup>+</sup> challenge. <i>New Journal of Physics</i> , <b>2016</b> , 18, 073026	2.9	10
24	Efficient Amino Acid Conformer Search with Bayesian Optimization. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 1955-1966	6.4	9
23	Theory of optical excitations in dipole-coupled hybrid molecule-semiconductor layers: Coupling of a molecular resonance to semiconductor continuum states. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	7
22	Quantum embedding theory in the screened Coulomb interaction: Combining configuration interaction with GW/BSE. <i>Physical Review Materials</i> , <b>2019</b> , 3,	3.2	7
21	Detecting stable adsorbates of (1)-camphor on Cu(111) with Bayesian optimization. <i>Beilstein Journal of Nanotechnology</i> , <b>2020</b> , 11, 1577-1589	3	7
20	Real-time time-dependent density functional theory implementation of electronic circular dichroism applied to nanoscale metal-organic clusters. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 114102	3.9	6
19	Materials structure genealogy and high-throughput topological classification of surfaces and 2D materials. <i>Npj Computational Materials</i> , <b>2018</b> , 4,	10.9	6
18	Machine Learning: Deep Learning Spectroscopy: Neural Networks for Molecular Excitation Spectra (Adv. Sci. 9/2019). <i>Advanced Science</i> , <b>2019</b> , 6, 1970053	13.6	5
17	Optical Properties of Silver-Mediated DNA from Molecular Dynamics and Time Dependent Density Functional Theory. <i>International Journal of Molecular Sciences</i> , <b>2018</b> , 19,	6.3	5
16	Electron-phonon coupling in d-electron solids: A temperature-dependent study of rutile TiO <sub>2</sub> by first-principles theory and two-photon photoemission. <i>Physical Review Research</i> , <b>2019</b> , 1,	3.9	5
15	Database-driven high-throughput study of coating materials for hybrid perovskites. <i>New Journal of Physics</i> , <b>2019</b> , 21, 083018	2.9	4

14	Raman study of 2,7-bis(biphenyl-4-yl)-2,2',7,7'-ditertbutyl-9,9'-spirobifluorene adsorbed on oxide surfaces. <i>Chemical Physics Letters</i> , <b>2013</b> , 584, 74-78	2.5	3
13	Gold diggers: Altered reconstruction of the gold surface by physisorbed aromatic oligomers. <i>Physical Review Materials</i> , <b>2019</b> , 3,	3.2	3
12	Formation of graphene atop a Si adlayer on the C-face of SiC. <i>Physical Review Materials</i> , <b>2019</b> , 3,	3.2	3
11	Improved One-Shot Total Energies from the Linearized GW Density Matrix. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 2126-2136	6.4	3
10	Multi-scale model for the structure of hybrid perovskites: analysis of charge migration in disordered MAPbI <sub>3</sub> structures. <i>New Journal of Physics</i> , <b>2018</b> , 20, 103013	2.9	3
9	Assessing the $\Gamma$ Approach: Beyond with Hedin's Full Second-Order Self-Energy Contribution. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 5140-5154	6.4	3
8	Theory of Excitation Transfer between Two-Dimensional Semiconductor and Molecular Layers. <i>Physical Review Applied</i> , <b>2018</b> , 9,	4.3	2
7	Electronic Characterization of a Charge-Transfer Complex Monolayer on Graphene. <i>ACS Nano</i> , <b>2021</b> , 15, 9945-9954	16.7	2
6	Lithium-Ion Battery Technology for Voltage Control of Perpendicular Magnetization. <i>Advanced Functional Materials</i> , 2113118	15.6	2
5	All-Electron BSE@ Method for $\pi$ -Edge Core Electron Excitation Energies.. <i>Journal of Chemical Theory and Computation</i> , <b>2022</b> ,	6.4	1
4	Integrating Bayesian Inference with Scanning Probe Experiments for Robust Identification of Surface Adsorbate Configurations. <i>Advanced Functional Materials</i> , <b>2021</b> , 31, 2010853	15.6	1
3	Atomic and electronic structure of cesium lead triiodide surfaces. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 074712	3.9	1
2	Machine learning as a tool to engineer microstructures: Morphological prediction of tannin-based colloids using Bayesian surrogate models.. <i>MRS Bulletin</i> , <b>2022</b> , 47, 1-9	3.2	1
1	Integrating Bayesian Inference with Scanning Probe Experiments for Robust Identification of Surface Adsorbate Configurations (Adv. Funct. Mater. 32/2021). <i>Advanced Functional Materials</i> , <b>2021</b> , 31, 2170235	15.6	