Fabien Bruneval

List of Publications by Year
in descending order

64 papers	6,756 citations	126907 33 h-index	106344 65 g-index
67 all docs	67 docs citations	67 times ranked	6377 citing authors

#	Article	IF	Citations
1	ABINIT: First-principles approach to material and nanosystem properties. Computer Physics Communications, 2009, 180, 2582-2615.	7.5	2,297
2	Recent developments in the ABINIT software package. Computer Physics Communications, 2016, 205, 106-131.	7.5	662
3	The Abinitproject: Impact, environment and recent developments. Computer Physics Communications, 2020, 248, 107042.	7.5	369
4	Effect of self-consistency on quasiparticles in solids. Physical Review B, 2006, 74, .	3.2	230
5	Benchmarking the Starting Points of the GW Approximation for Molecules. Journal of Chemical Theory and Computation, 2013, 9, 324-329.	5.3	206
6	Understanding Correlations in Vanadium Dioxide from First Principles. Physical Review Letters, 2007, 99, 266402.	7.8	198
7	Accurate<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>self-energies in a plane-wave basis using only a few empty states: Towards large systems. Physical Review B, 2008, 78, .	3.2	194
8	ABINIT: Overview and focus on selected capabilities. Journal of Chemical Physics, 2020, 152, 124102.	3.0	179
9	Point defect modeling in materials: Couplingab initioand elasticity approaches. Physical Review B, 2013, 88, .	3.2	158
10	molgw 1: Many-body perturbation theory software for atoms, molecules, and clusters. Computer Physics Communications, 2016, 208, 149-161.	7.5	139
11	A systematic benchmark of the ab initio Bethe-Salpeter equation approach for low-lying optical excitations of small organic molecules. Journal of Chemical Physics, 2015, 142, 244101.	3.0	137
12	Many-Body Perturbation Theory Using the Density-Functional Concept: Beyond theGWApproximation. Physical Review Letters, 2005, 94, 186402.	7.8	126
13	A Molecular Dynamics Study of the Early Stages of Calcium Carbonate Growth. Journal of Physical Chemistry B, 2009, 113, 11680-11687.	2.6	116
14	Exchange and Correlation Effects in Electronic Excitations ofCu2O. Physical Review Letters, 2006, 97, 267601.	7.8	114
15	Ionization energy of atoms obtained from GW self-energy or from random phase approximation total energies. Journal of Chemical Physics, 2012, 136, 194107.	3.0	96
16	Understanding and correcting the spurious interactions in charged supercells. Physical Review B, 2011, 84, .	3.2	89
17	Effects of Electronic and Lattice Polarization on the Band Structure of Delafossite Transparent Conductive Oxides. Physical Review Letters, 2010, 104, 136401.	7.8	88
18	An assessment of low-lying excitation energies and triplet instabilities of organic molecules with an ab initio Bethe-Salpeter equation approach and the Tamm-Dancoff approximation. Journal of Chemical Physics, 2017, 146, 194108.	3.0	81

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19	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:math>Approximation of the Many-Body Problem and Changes in the Particle Number. Physical Review Letters, 2009, 103, 176403.	7.8	77
20	Evaluating the GW Approximation with CCSD(T) for Charged Excitations Across the Oligoacenes. Journal of Chemical Theory and Computation, 2016, 12, 2834-2842.	5.3	71
21	Direct Comparison of Many-Body Methods for Realistic Electronic Hamiltonians. Physical Review X, 2020, 10, .	8.9	68
22	Molecular Dynamics Study of the Solvation of Calcium Carbonate in Water. Journal of Physical Chemistry B, 2007, 111, 12219-12227.	2.6	66
23	TDDFT from molecules to solids: The role of long-range interactions. International Journal of Quantum Chemistry, 2005, 102, 684-701.	2.0	65
24	Screened Coulomb interaction calculations: cRPA implementation and applications to dynamical screening and self-consistency in uranium dioxide and cerium. Physical Review B, 2014, 89, .	3.2	61
25	Dynamic structure factor and dielectric function of silicon for finite momentum transfer: Inelastic x-ray scattering experiments andab initiocalculations. Physical Review B, 2010, 81, .	3.2	50
26	Comment on â€œQuantum Confinement and Electronic Properties of Silicon Nanowiresâ€• Physical Review Letters, 2005, 94, 219701; author reply 219702.	7.8	43
27	Signatures of Short-Range Many-Body Effects in the Dielectric Function of Silicon for Finite Momentum Transfer. Physical Review Letters, 2006, 97, 237602.	7.8	40
28	Ab initioelectronic stopping power of protons in bulk materials. Physical Review B, 2016, 93, .	3.2	40
29	Pressure, relaxation volume, and elastic interactions in charged simulation cells. Physical Review B, 2015, 91, .	3.2	38
30	GW and Bethe-Salpeter study of small water clusters. Journal of Chemical Physics, 2016, 144, 034109.	3.0	38
31	Range-Separated Approach to the RPA Correlation Applied to the van der Waals Bond and to Diffusion of Defects. Physical Review Letters, 2012, 108, 256403.	7.8	37
32	Reproducibility in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e1825" altimg="si271.svg"><mml:mrow><mml:msub><mml:mrow><mml:mi>G</mml:mi></mml:mrow><mml:mrow><mml:mn>0</mml:mn></ calculations for solids. Computer Physics Communications, 2020, 255, 107242.	7.5	36
33	Benchmarking the GW Approximation and Betheâ€“Salpeter Equation for Groups IB and IIB Atoms and Monoxides. Journal of Chemical Theory and Computation, 2017, 13, 2135-2146.	5.3	34
34	Energetics and metastability of the silicon vacancy in cubic SiC. Physical Review B, 2011, 83, .	3.2	33
35	Beyond time-dependent exact exchange: The need for long-range correlation. Journal of Chemical Physics, 2006, 124, 144113.	3.0	32
36	ComprehensiveAb InitioStudy of Doping in Bulk ZnO with Group-V Elements. Physical Review Applied, 2014, 1, .	3.8	32

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37	The GW Miracle in Many-Body Perturbation Theory for the Ionization Potential of Molecules. Frontiers in Chemistry, 2021, 9, 749779.	3.6	32
38	Electronic stopping power from time-dependent density-functional theory in Gaussian basis. European Physical Journal B, 2018, 91, 1.	1.5	28
39	Quasiparticle Self-Consistent GW Method for the Spectral Properties of Complex Materials. Topics in Current Chemistry, 2014, 347, 99-135.	4.0	27
40	Consistent treatment of charged systems within periodic boundary conditions: The projector augmented-wave and pseudopotential methods revisited. Physical Review B, 2014, 89, .	3.2	25
41	Optimized virtual orbital subspace for faster GW calculations in localized basis. Journal of Chemical Physics, 2016, 145, 234110.	3.0	24
42	Electronic excitations: Ab initio calculations of electronic spectra and application to zirconia ZrO2, titania TiO2 and cuprous oxide Cu2O. Computational Materials Science, 2007, 38, 482-493.	3.0	22
43	p-type doping and codoping of ZnO based on nitrogen is ineffective: An ab initio clue. Applied Physics Letters, 2010, 97, 042108.	3.3	22
44	Lattice constant in nonstoichiometric uranium dioxide from first principles. Physical Review Materials, 2018, 2, .	2.4	22
45	Direct observation of Al-doping-induced electronic states in the valence band and band gap of ZnO films. Physical Review B, 2011, 84, .	3.2	18
46	Methodological aspects of the GW calculation of the carbon vacancy in 3C-SiC. Nuclear Instruments & Methods in Physics Research B, 2012, 277, 77-79.	1.4	17
47	Influence of vibrational entropy on the concentrations of oxygen interstitial clusters and uranium vacancies in nonstoichiometric <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">U</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review Materials, 2018, 2, .	2.4	15
48	Ab initioformation volume of charged defects. Physical Review B, 2012, 86, .	3.2	14
49	Effects of quantum confinement on excited state properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mi>initio</mml:i>many-body perturbation theory. Physical Review B, 2016, 94, .	3.2	14
50	Extrapolating Unconverged GW Energies up to the Complete Basis Set Limit with Linear Regression. Journal of Chemical Theory and Computation, 2020, 16, 4399-4407.	5.3	14
51	Coupling Natural Orbital Functional Theory and Many-Body Perturbation Theory by Using Nondynamically Correlated Canonical Orbitals. Journal of Chemical Theory and Computation, 2021, 17, 7562-7574.	5.3	14
52	Assessment of the Linearized GW Density Matrix for Molecules. Journal of Chemical Theory and Computation, 2019, 15, 4069-4078.	5.3	13
53	Quantitative electronic stopping power from localized basis set. Physical Review B, 2020, 101, .	3.2	13
54	New Lennard-Jones metastable phase. Journal of Chemical Physics, 2008, 129, 026101.	3.0	10

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55	First-Principles Approach to the Conductance of Covalently Bound Molecular Junctions. Journal of Physical Chemistry C, 2019, 123, 6379-6387.	3.1	10
56	Photoelectron spectra of copper oxide cluster anions from first principles methods. Journal of Chemical Physics, 2018, 149, 064306.	3.0	8
57	Formation and Migration Energy of Native Defects in Silicon Carbide from First Principles: An Overview. Defect and Diffusion Forum, 0, 323-325, 11-18.	0.4	7
58	Systematic defect donor levels in III-V and II-VI semiconductors revealed by hybrid functional density-functional theory. Physical Review B, 2015, 92, .	3.2	7
59	Partial Molar Volumes of Aqua Ions from First Principles. Journal of Chemical Theory and Computation, 2017, 13, 3427-3431.	5.3	7
60	Improved density matrices for accurate molecular ionization potentials. Physical Review B, 2019, 99, .	3.2	7
61	Improved One-Shot Total Energies from the Linearized GW Density Matrix. Journal of Chemical Theory and Computation, 2021, 17, 2126-2136.	5.3	7
62	Optical Properties of Saturated and Unsaturated Carbonyl Defects in Polyethylene. Journal of Physical Chemistry B, 2018, 122, 2023-2030.	2.6	5
63	AbÂInitio Prediction of a Negative Barkas Coefficient for Slow Protons and Antiprotons in LiF. Physical Review Letters, 2022, 128, 043401.	7.8	5
64	Assessment of atomistic data for predicting the phase diagram and defect thermodynamics. The example of non-stoichiometric uranium dioxide. Journal of Nuclear Materials, 2022, 569, 153864.	2.7	4