Fabien Tran

List of Publications by Year
in descending order

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63 papers	10,862 citations	126907 33 h-index	114465 63 g-index
66 all docs	66 docs citations	66 times ranked	8784 citing authors

#	Article	IF	Citations
1	Accurate Band Gaps of Semiconductors and Insulators with a Semilocal Exchange-Correlation Potential. Physical Review Letters, 2009, 102, 226401.	7.8	4,279
2	WIEN2k: An APW+lo program for calculating the properties of solids. Journal of Chemical Physics, 2020, 152, 074101.	3.0	1,185
3	Merits and limits of the modified Becke-Johnson exchange potential. Physical Review B, 2011, 83, .	3.2	743
4	Calculation of the lattice constant of solids with semilocal functionals. Physical Review B, 2009, 79, .	3.2	709
5	Improving the modified Becke-Johnson exchange potential. Physical Review B, 2012, 85, .	3.2	552
6	Hybrid exchange-correlation energy functionals for strongly correlated electrons: Applications to transition-metal monoxides. Physical Review B, 2006, 74, .	3.2	309
7	Performance on molecules, surfaces, and solids of the Wu-Cohen GGA exchange-correlation energy functional. Physical Review B, 2007, 75, .	3.2	306
8	Towards efficient band structure and effective mass calculations for III-V direct band-gap semiconductors. Physical Review B, 2010, 82, .	3.2	279
9	Band gap calculations with Beckeâ€“Johnson exchange potential. Journal of Physics Condensed Matter, 2007, 19, 196208.	1.8	195
10	Rungs 1 to 4 of DFT Jacobâ€™s ladder: Extensive test on the lattice constant, bulk modulus, and cohesive energy of solids. Journal of Chemical Physics, 2016, 144, 204120.	3.0	191
11	Implementation of screened hybrid functionals based on the Yukawa potential within the LAPW basis set. Physical Review B, 2011, 83, .	3.2	159
12	Exchange-correlation functionals for band gaps of solids: benchmark, reparametrization and machine learning. Npj Computational Materials, 2020, 6, .	8.7	156
13	Large-Scale Benchmark of Exchangeâ€“Correlation Functionals for the Determination of Electronic Band Gaps of Solids. Journal of Chemical Theory and Computation, 2019, 15, 5069-5079.	5.3	151
14	Importance of the Kinetic Energy Density for Band Gap Calculations in Solids with Density Functional Theory. Journal of Physical Chemistry A, 2017, 121, 3318-3325.	2.5	126
15	Link between the kinetic- and exchange-energy functionals in the generalized gradient approximation. International Journal of Quantum Chemistry, 2002, 89, 441-446.	2.0	97
16	Gradient-free and gradient-dependent approximations in the total energy bifunctional for weakly overlapping electron densities. Journal of Chemical Physics, 2003, 118, 2072-2080.	3.0	77
17	Hybrid functionals for solids with an optimized Hartreeâ€“Fock mixing parameter. Journal of Physics Condensed Matter, 2013, 25, 435503.	1.8	74
18	Insight into the performance of GGA functionals for solid-state calculations. Physical Review B, 2009, 80, .	3.2	72

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19	Assessment of DFT functionals with NMR chemical shifts. Physical Review B, 2013, 87, .	3.2	72
20	Nonlocal van der Waals functionals for solids: Choosing an appropriate one. Physical Review Materials, 2019, 3, .	2.4	65
21	Efficient and accurate calculation of band gaps of halide perovskites with the Tran-Blaha modified Becke-Johnson potential. Physical Review B, 2019, 99, .	3.2	61
22	Physisorption of Molecular Hydrogen on Polycyclic Aromatic Hydrocarbons:â€‰ A Theoretical Study. Journal of Physical Chemistry B, 2002, 106, 8689-8696.	2.6	54
23	Site-selective adsorption of phthalocyanine on h-BN/Rh(111) nanomesh. Physical Chemistry Chemical Physics, 2014, 16, 12374-12384.	2.8	47
24	Assessment of the GLLB-SC potential for solid-state properties and attempts for improvement. Physical Review Materials, 2018, 2, .	2.4	44
25	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>F</mml:mi></mml:math>center in lithium fluoride revisited: Comparison of solid-state physics and quantum-chemistry approaches. Physical Review B, 2014, 89, .	3.2	43
26	Nonlocal van der Waals functionals: The case of rare-gas dimers and solids. Journal of Chemical Physics, 2013, 138, 204103.	3.0	42
27	Theoretical Study of the Benzene Dimer by the Density-Functional-Theory Formalism Based on Electron-Density Partitioning. Helvetica Chimica Acta, 2001, 84, 1489-1503.	1.6	41
28	Semilocal exchange-correlation potentials for solid-state calculations: Current status and future directions. Journal of Applied Physics, 2019, 126, .	2.5	41
29	Systematic investigation of a family of gradient-dependent functionals for solids. Physical Review B, 2010, 81, .	3.2	36
30	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>PBE</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math>calculat of the Jahn-Teller effect in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Pr</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2008, 77, .	3.2	35
31	The small unit cell reconstructions of SrTiO3(111). Surface Science, 2009, 603, 2179-2187.	1.9	33
32	Comparison between exact and semilocal exchange potentials: An all-electron study for solids. Physical Review B, 2015, 91, .	3.2	33
33	Calculating energy loss spectra of NiO: Advantages of the modified Becke-Johnson potential. Physical Review B, 2012, 85, .	3.2	28
34	Limitations of the DFTâ€“1/2 method for covalent semiconductors and transition-metal oxides. Physical Review B, 2019, 99, .	3.2	27
35	Shortcomings of meta-GGA functionals when describing magnetism. Physical Review B, 2020, 102, .	3.2	27
36	Bandgap of two-dimensional materials: Thorough assessment of modern exchangeâ€“correlation functionals. Journal of Chemical Physics, 2021, 155, 104103.	3.0	26

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37	Force calculation for orbital-dependent potentials with FP-(L)APW+lo basis sets. Computer Physics Communications, 2008, 179, 784-790.	7.5	25
38	Validation of Pseudopotential Calculations for the Electronic Band Gap of Solids. Journal of Chemical Theory and Computation, 2020, 16, 3620-3627.	5.3	25
39	The role of density functional theory in chemistry: Some historical landmarks and applications to zeolites. Computational and Theoretical Chemistry, 2006, 762, 1-7.	1.5	24
40	Application of screened hybrid functionals to the bulk transition metals Rh, Pd, and Pt. Physical Review B, 2012, 86, .	3.2	24
41	On the accuracy of the non-self-consistent calculation of the electronic structure of solids with hybrid functionals. Physics Letters, Section A: General, Atomic and Solid State Physics, 2012, 376, 879-882.	2.1	23
42	On the importance of local orbitals using second energy derivatives for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" id="mml66" display="inline" overflow="scroll" altimg="si66.gif"><mml:mi>d</mml:mi></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" id="mml67" display="inline" overflow="scroll" altimg="si67.gif"><mml:mi>f</mml:mi></mml:math> electrons. Computer Physics Communications, 2017, 220, 230-238.	7.5	22
43	Perturbation approach to ab initio effective mass calculations. Computer Physics Communications, 2021, 261, 107648.	7.5	21
44	Efficient Band Structure Calculation of Two-Dimensional Materials from Semilocal Density Functionals. Journal of Physical Chemistry C, 2021, 125, 11206-11215.	3.1	19
45	Ï€-Stacking Behavior of Selected Nitrogen-Containing PAHs. Journal of Physical Chemistry A, 2004, 108, 9155-9160.	2.5	17
46	Semilocal Approximations for the Kinetic Energy. Recent Advances in Computational, 2013, , 429-442.	0.8	17
47	How Close Are the Slater and Beckeâ€“Roussel Potentials in Solids?. Journal of Chemical Theory and Computation, 2015, 11, 4717-4726.	5.3	17
48	Orbital-free approximations to the kinetic-energy density in exchange-correlation MGGA functionals: Tests on solids. Journal of Chemical Physics, 2018, 149, 144105.	3.0	17
49	Simple way to apply nonlocal van der Waals functionals within all-electron methods. Physical Review B, 2017, 96, .	3.2	16
50	Comparative study of the PBE and SCAN functionals: The particular case of alkali metals. Journal of Chemical Physics, 2019, 150, 164119.	3.0	16
51	Approximations to the exact exchange potential: KLI versus semilocal. Physical Review B, 2016, 94, .	3.2	14
52	Nonmagnetic and ferromagnetic fcc cerium studied with one-electron methods. Physical Review B, 2014, 89, .	3.2	13
53	DFT study of the electronic properties and the cubic to tetragonal phase transition in RbCaF3. Physical Review Materials, 2018, 2, .	2.4	13
54	On the calculation of the bandgap of periodic solids with MGGA functionals using the total energy. Journal of Chemical Physics, 2019, 151, 161102.	3.0	10

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55	Introduction of the explicit long-range nonlocality as an alternative to the gradient expansion approximation for the kinetic-energy functional. Chemical Physics Letters, 2002, 360, 209-216.	2.6	9
56	Theoretical study of neutral and cationic complexes involving phenol. International Journal of Quantum Chemistry, 2005, 101, 854-859.	2.0	9
57	Implementation of self-consistent MGGA functionals in augmented plane wave based methods. Physical Review B, 2022, 105, .	3.2	4
58	What is the optimal mGGA exchange functional for solids?. Journal of Chemical Physics, 2022, 157, .	3.0	3
59	One-Electron Equations for Embedded Electron Density and Their Applications to Study Electronic Structure of Atoms and Molecules in Condensed Phase. Chimia, 2005, 59, 488-492.	0.6	2
60	Density Functional Theory Study of Metal and Metal-Oxide Nucleation and Growth on the Anatase TiO2(101) Surface. Computation, 2021, 9, 125.	2.0	2
61	Approximation to the classical Coulomb energy for atoms. Physics Letters, Section A: General, Atomic and Solid State Physics, 2003, 310, 177-181.	2.1	1
62	Density analysis for estimating the degree of on-site correlation on transition-metal atoms in extended systems. Physical Review B, 2021, 104, .	3.2	0
63	Similarity Clustering for Representative Sets of Inorganic Solids for Density Functional Testing. Journal of Chemical Theory and Computation, 2022, 18, 441-447.	5.3	0