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	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
2	Implementation of self-consistent MGGA functionals in augmented plane wave based methods. Physical Review B, 2022, 105, .	3.2	4
3	What is the optimal mGGA exchange functional for solids?. Journal of Chemical Physics, 2022, 157, .	3.0	3
4	Perturbation approach to ab initio effective mass calculations. Computer Physics Communications, 2021, 261, 107648.	7.5	21
5	Efficient Band Structure Calculation of Two-Dimensional Materials from Semilocal Density Functionals. Journal of Physical Chemistry C, 2021, 125, 11206-11215.	3.1	19
6	Bandgap of two-dimensional materials: Thorough assessment of modern exchangeâ€“correlation functionals. Journal of Chemical Physics, 2021, 155, 104103.	3.0	26
7	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
8	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
9	Shortcomings of meta-GGA functionals when describing magnetism. Physical Review B, 2020, 102, .	3.2	27
10	Exchange-correlation functionals for band gaps of solids: benchmark, reparametrization and machine learning. Npj Computational Materials, 2020, 6, .	8.7	156
11	Validation of Pseudopotential Calculations for the Electronic Band Gap of Solids. Journal of Chemical Theory and Computation, 2020, 16, 3620-3627.	5.3	25
12	WIEN2k: An APW+lo program for calculating the properties of solids. Journal of Chemical Physics, 2020, 152, 074101.	3.0	1,185
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	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
15	Semilocal exchange-correlation potentials for solid-state calculations: Current status and future directions. Journal of Applied Physics, 2019, 126, .	2.5	41
16	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
17	Comparative study of the PBE and SCAN functionals: The particular case of alkali metals. Journal of Chemical Physics, 2019, 150, 164119.	3.0	16
18	Limitations of the DFTâ€“1/2 method for covalent semiconductors and transition-metal oxides. Physical Review B, 2019, 99, .	3.2	27

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19	Nonlocal van der Waals functionals for solids: Choosing an appropriate one. Physical Review Materials, 2019, 3, .	2.4	65
20	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
21	Assessment of the GLLB-SC potential for solid-state properties and attempts for improvement. Physical Review Materials, 2018, 2, .	2.4	44
22	DFT study of the electronic properties and the cubic to tetragonal phase transition in RbCaF3. Physical Review Materials, 2018, 2, .	2.4	13
23	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
24	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
25	Simple way to apply nonlocal van der Waals functionals within all-electron methods. Physical Review B, 2017, 96, .	3.2	16
26	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
27	Approximations to the exact exchange potential: KLI versus semilocal. Physical Review B, 2016, 94, .	3.2	14
28	Comparison between exact and semilocal exchange potentials: An all-electron study for solids. Physical Review B, 2015, 91, .	3.2	33
29	How Close Are the Slater and Beckeâ€“Roussel Potentials in Solids?. Journal of Chemical Theory and Computation, 2015, 11, 4717-4726.	5.3	17
30	Nonmagnetic and ferromagnetic fcc cerium studied with one-electron methods. Physical Review B, 2014, 89, .	3.2	13
31	Site-selective adsorption of phthalocyanine on h-BN/Rh(111) nanomesh. Physical Chemistry Chemical Physics, 2014, 16, 12374-12384.	2.8	47
32	<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
33	Assessment of DFT functionals with NMR chemical shifts. Physical Review B, 2013, 87, .	3.2	72
34	Nonlocal van der Waals functionals: The case of rare-gas dimers and solids. Journal of Chemical Physics, 2013, 138, 204103.	3.0	42
35	Semilocal Approximations for the Kinetic Energy. Recent Advances in Computational, 2013, , 429-442.	0.8	17
36	Hybrid functionals for solids with an optimized Hartreeâ€“Fock mixing parameter. Journal of Physics Condensed Matter, 2013, 25, 435503.	1.8	74

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37	Calculating energy loss spectra of NiO: Advantages of the modified Becke-Johnson potential. Physical Review B, 2012, 85, .	3.2	28
38	Application of screened hybrid functionals to the bulk transition metals Rh, Pd, and Pt. Physical Review B, 2012, 86, .	3.2	24
39	Improving the modified Becke-Johnson exchange potential. Physical Review B, 2012, 85, .	3.2	552
40	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
41	Merits and limits of the modified Becke-Johnson exchange potential. Physical Review B, 2011, 83, .	3.2	743
42	Implementation of screened hybrid functionals based on the Yukawa potential within the LAPW basis set. Physical Review B, 2011, 83, .	3.2	159
43	Systematic investigation of a family of gradient-dependent functionals for solids. Physical Review B, 2010, 81, .	3.2	36
44	Towards efficient band structure and effective mass calculations for III-V direct band-gap semiconductors. Physical Review B, 2010, 82, .	3.2	279
45	Insight into the performance of GGA functionals for solid-state calculations. Physical Review B, 2009, 80, .	3.2	72
46	The small unit cell reconstructions of SrTiO3(111). Surface Science, 2009, 603, 2179-2187.	1.9	33
47	Accurate Band Gaps of Semiconductors and Insulators with a Semilocal Exchange-Correlation Potential. Physical Review Letters, 2009, 102, 226401.	7.8	4,279
48	Calculation of the lattice constant of solids with semilocal functionals. Physical Review B, 2009, 79, .	3.2	709
49	Force calculation for orbital-dependent potentials with FP-(L)APW+lo basis sets. Computer Physics Communications, 2008, 179, 784-790.	7.5	25
50	<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
51	Band gap calculations with Beckeâ€“Johnson exchange potential. Journal of Physics Condensed Matter, 2007, 19, 196208.	1.8	195
52	Performance on molecules, surfaces, and solids of the Wu-Cohen GGA exchange-correlation energy functional. Physical Review B, 2007, 75, .	3.2	306
53	Hybrid exchange-correlation energy functionals for strongly correlated electrons: Applications to transition-metal monoxides. Physical Review B, 2006, 74, .	3.2	309
54	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

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55	Theoretical study of neutral and cationic complexes involving phenol. International Journal of Quantum Chemistry, 2005, 101, 854-859.	2.0	9
56	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
57	Ï€-Stacking Behavior of Selected Nitrogen-Containing PAHs. Journal of Physical Chemistry A, 2004, 108, 9155-9160.	2.5	17
58	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
59	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
60	Physisorption of Molecular Hydrogen on Polycyclic Aromatic Hydrocarbons:â€‰ A Theoretical Study. Journal of Physical Chemistry B, 2002, 106, 8689-8696.	2.6	54
61	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
62	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
63	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