Thierry Deutsch

List of Publications by Year
in descending order

51	6,620	159585 30	182427 51
papers	citations	h-index	g-index

55	55	55	8448
all docs	docs citations	times ranked	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	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
3	CO Oxidation on Pt(111): AnAb InitioDensity Functional Theory Study. Physical Review Letters, 1998, 80, 3650-3653.	7.8	675
4	Daubechies wavelets as a basis set for density functional pseudopotential calculations. Journal of Chemical Physics, 2008, 129, 014109.	3.0	289
5	Efficient solution of Poissonâ€™s equation with free boundary conditions. Journal of Chemical Physics, 2006, 125, 074105.	3.0	176
6	First-Principles Calculations of the Ideal Cleavage Energy of Bulk Niobium(111)/Î±-Alumina(0001) Interfaces. Physical Review Letters, 1999, 82, 1510-1513.	7.8	174
7	Accurate and efficient linear scaling DFT calculations with universal applicability. Physical Chemistry Chemical Physics, 2015, 17, 31360-31370.	2.8	158
8	Daubechies wavelets for linear scaling density functional theory. Journal of Chemical Physics, 2014, 140, 204110.	3.0	140
9	A Fourfold Coordinated Point Defect in Silicon. Physical Review Letters, 2002, 88, 235501.	7.8	102
10	Efficient and accurate three-dimensional Poisson solver for surface problems. Journal of Chemical Physics, 2007, 127, 054704.	3.0	102
11	Assessment of noncollinear spin-flip Tammâ€“Dancoff approximation time-dependent density-functional theory for the photochemical ring-opening of oxirane. Physical Chemistry Chemical Physics, 2010, 12, 12811.	2.8	99
12	Challenges in large scale quantum mechanical calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1290.	14.6	98
13	Short-Range to Long-Range Charge-Transfer Excitations in the Zincbacteriochlorin-Bacteriochlorin Complex: A Bethe-Salpeter Study. Physical Review Letters, 2012, 109, 167801.	7.8	97
14	Norm-conserving pseudopotentials with chemical accuracy compared to all-electron calculations. Journal of Chemical Physics, 2013, 138, 104109.	3.0	95
15	Density functional theory calculation on many-cores hybrid central processing unit-graphic processing unit architectures. Journal of Chemical Physics, 2009, 131, 034103.	3.0	87
16	Optimized energy landscape exploration using the ab initio based activation-relaxation technique. Journal of Chemical Physics, 2011, 135, 034102.	3.0	81
17	Quantitative analysis of the deformation and chemical profiles of strained multilayers. Ultramicroscopy, 1994, 56, 94-107.	1.9	60
18	Flexibilities of wavelets as a computational basis set for large-scale electronic structure calculations. Journal of Chemical Physics, 2020, 152, 194110.	3.0	60

#	Article	IF	Citations
19	Daubechies wavelets for high performance electronic structure calculations: The BigDFT project. Comptes Rendus - Mecanique, 2011, 339, 149-164.	2.1	53
20	Many-body Green's function study of coumarins for dye-sensitized solar cells. Physical Review B, 2012, 86, .	3.2	51
21	Phase diagram, structure, and magnetic properties of the Ge-Mn system: A first-principles study. Physical Review B, 2011, 83, .	3.2	47
22	Structural metastability of endohedral silicon fullerenes. Physical Review B, 2010, 81, .	3.2	39
23	Toward Fast and Accurate Evaluation of Charge On-Site Energies and Transfer Integrals in Supramolecular Architectures Using Linear Constrained Density Functional Theory (CDFT)-Based Methods. Journal of Chemical Theory and Computation, 2015, 11, 2077-2086.	5.3	38
24	First-principles prediction of stable SiC cage structures and their synthesis pathways. Physical Review B, 2010, 82, .	3.2	37
25	Low-energy boron fullerenes: Role of disorder and potential synthesis pathways. Physical Review B, 2011, 83, .	3.2	37
26	Germanium diffusion mechanisms in silicon from first principles. Physical Review B, 2007, 75, .	3.2	33
27	Revisiting the domain model for lithium intercalated graphite. Applied Physics Letters, 2013, 103, .	3.3	33
28	Exploring approximations to theGWself-energy ionic gradients. Physical Review B, 2015, 91, .	3.2	32
29	Electronâ€“phonon coupling and charge-transfer excitations in organic systems from many-body perturbation theory. Journal of Materials Science, 2012, 47, 7472-7481.	3.7	31
30	Ab initiocalculation of the binding energy of impurities in semiconductors: Application to Si nanowires. Physical Review B, 2010, 81, .	3.2	30
31	Computer simulation of Au(001)/Ni multilayers: comparison with experiments. Journal of Physics Condensed Matter, 1995, 7, 6407-6421.	1.8	25
32	Metallofullerenes as fuel cell electrocatalysts: A theoretical investigation of adsorbates on C59Pt. Physical Chemistry Chemical Physics, 2010, 12, 9406.	2.8	23
33	Magnetic anisotropy in icosahedral cobalt clusters. Journal of Magnetism and Magnetic Materials, 2007, 308, 296-304.	2.3	21
34	SERENADE: safer and ecodesign research and education applied to nanomaterial development, the new generation of materials safer by design. Environmental Science: Nano, 2017, 4, 526-538.	4.3	21
35	Linear scaling relaxation of the atomic positions in nanostructures. Physical Review B, 2001, 64, .	3.2	20
36	An efficient 3-dim FFT for plane wave electronic structure calculations on massively parallel machines composed ofÂmultiprocessor nodes. Computer Physics Communications, 2003, 154, 105-110.	7.5	17

#	Article	IF	Citations
37	Structure determination of the () reconstructed Î±-Al2O3(0001). Surface Science, 2002, 505, L215-L221.	1.9	16
38	Wavelet-based linear-response time-dependent density-functional theory. Chemical Physics, 2012, 402, 29-40.	1.9	16
39	Fragment approach to constrained density functional theory calculations using Daubechies wavelets. Journal of Chemical Physics, 2015, 142, 234105.	3.0	16
40	On the stability of (001) Au/Ni artificially modulated structures grown by MBE. Journal of Crystal Growth, 2001, 222, 685-691.	1.5	11
41	First principles prediction of the metastability of the Ge2Mn phase and its synthesis pathways. Applied Physics Letters, 2010, 96, 231904.	3.3	11
42	Accurate complex scaling of three dimensional numerical potentials. Journal of Chemical Physics, 2013, 138, 204111.	3.0	9
43	Multipole-preserving quadratures for the discretization of functions in real-space electronic structure calculations. Physical Chemistry Chemical Physics, 2015, 17, 31582-31591.	2.8	9
44	BOAST. International Journal of High Performance Computing Applications, 2018, 32, 28-44.	3.7	8
45	Fullerene-Based Materials as Catalysts for Fuel Cells. ECS Transactions, 2010, 25, 1-6.	0.5	7
46	Wavelets for electronic structure calculations. Ã‰cole ThÃ©matique De La SociÃ©tÃ© FranÃ§aise De La Neutronique, 2011, 12, 33-76.	0.2	5
47	Organizing Software Growth and Distributed Development: The Case of Abinit. Computing in Science and Engineering, 2011, 13, 62-69.	1.2	4
48	Stability and internal stresses in Au(001)/Ni multilayers. Journal of Physics Condensed Matter, 2003, 15, 1813-1826.	1.8	2
49	Oxygen in silicon: Switch in the diffusion-mediated mechanism. Physical Review B, 2017, 96, .	3.2	2
50	Instrumental Data Management and Scientific Workflow Execution: the CEA Case Study. , 2019, , .		0
51	Wavelet-Based Density Functional Theory Calculation on Massively Parallel Hybrid Architectures. , 2011, , 133-151.		0