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	Flexibilities of wavelets as a computational basis set for large-scale electronic structure calculations. Journal of Chemical Physics, 2020, 152, 194110.	3.0	60
2	Instrumental Data Management and Scientific Workflow Execution: the CEA Case Study. , 2019, , .		0
3	BOAST. International Journal of High Performance Computing Applications, 2018, 32, 28-44.	3.7	8
4	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
5	Oxygen in silicon: Switch in the diffusion-mediated mechanism. Physical Review B, 2017, 96, .	3.2	2
6	Challenges in large scale quantum mechanical calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1290.	14.6	98
7	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
8	Exploring approximations to theGWself-energy ionic gradients. Physical Review B, 2015, 91, .	3.2	32
9	Fragment approach to constrained density functional theory calculations using Daubechies wavelets. Journal of Chemical Physics, 2015, 142, 234105.	3.0	16
10	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
11	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
12	Accurate and efficient linear scaling DFT calculations with universal applicability. Physical Chemistry Chemical Physics, 2015, 17, 31360-31370.	2.8	158
13	Daubechies wavelets for linear scaling density functional theory. Journal of Chemical Physics, 2014, 140, 204110.	3.0	140
14	Accurate complex scaling of three dimensional numerical potentials. Journal of Chemical Physics, 2013, 138, 204111.	3.0	9
15	Norm-conserving pseudopotentials with chemical accuracy compared to all-electron calculations. Journal of Chemical Physics, 2013, 138, 104109.	3.0	95
16	Revisiting the domain model for lithium intercalated graphite. Applied Physics Letters, 2013, 103, .	3.3	33
17	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
18	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

#	Article	IF	Citations
19	Many-body Green's function study of coumarins for dye-sensitized solar cells. Physical Review B, 2012, 86, .	3.2	51
20	Wavelet-based linear-response time-dependent density-functional theory. Chemical Physics, 2012, 402, 29-40.	1.9	16
21	Low-energy boron fullerenes: Role of disorder and potential synthesis pathways. Physical Review B, 2011, 83, .	3.2	37
22	Phase diagram, structure, and magnetic properties of the Ge-Mn system: A first-principles study. Physical Review B, 2011, 83, .	3.2	47
23	Organizing Software Growth and Distributed Development: The Case of Abinit. Computing in Science and Engineering, 2011, 13, 62-69.	1.2	4
24	Daubechies wavelets for high performance electronic structure calculations: The BigDFT project. Comptes Rendus - Mecanique, 2011, 339, 149-164.	2.1	53
25	Optimized energy landscape exploration using the ab initio based activation-relaxation technique. Journal of Chemical Physics, 2011, 135, 034102.	3.0	81
26	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
27	Wavelet-Based Density Functional Theory Calculation on Massively Parallel Hybrid Architectures. , 2011, , 133-151.		0
28	Fullerene-Based Materials as Catalysts for Fuel Cells. ECS Transactions, 2010, 25, 1-6.	0.5	7
29	First principles prediction of the metastability of the Ge2Mn phase and its synthesis pathways. Applied Physics Letters, 2010, 96, 231904.	3.3	11
30	Ab initiocalculation of the binding energy of impurities in semiconductors: Application to Si nanowires. Physical Review B, 2010, 81, .	3.2	30
31	First-principles prediction of stable SiC cage structures and their synthesis pathways. Physical Review B, 2010, 82, .	3.2	37
32	Structural metastability of endohedral silicon fullerenes. Physical Review B, 2010, 81, .	3.2	39
33	Metallofullerenes as fuel cell electrocatalysts: A theoretical investigation of adsorbates on C59Pt. Physical Chemistry Chemical Physics, 2010, 12, 9406.	2.8	23
34	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
35	ABINIT: First-principles approach to material and nanosystem properties. Computer Physics Communications, 2009, 180, 2582-2615.	7.5	2,297
36	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

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37	Daubechies wavelets as a basis set for density functional pseudopotential calculations. Journal of Chemical Physics, 2008, 129, 014109.	3.0	289
38	Efficient and accurate three-dimensional Poisson solver for surface problems. Journal of Chemical Physics, 2007, 127, 054704.	3.0	102
39	Germanium diffusion mechanisms in silicon from first principles. Physical Review B, 2007, 75, .	3.2	33
40	Magnetic anisotropy in icosahedral cobalt clusters. Journal of Magnetism and Magnetic Materials, 2007, 308, 296-304.	2.3	21
41	Efficient solution of Poissonâ€™s equation with free boundary conditions. Journal of Chemical Physics, 2006, 125, 074105.	3.0	176
42	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
43	Stability and internal stresses in Au(001)/Ni multilayers. Journal of Physics Condensed Matter, 2003, 15, 1813-1826.	1.8	2
44	A Fourfold Coordinated Point Defect in Silicon. Physical Review Letters, 2002, 88, 235501.	7.8	102
45	Structure determination of the () reconstructed Î±-Al2O3(0001). Surface Science, 2002, 505, L215-L221.	1.9	16
46	On the stability of (001) Au/Ni artificially modulated structures grown by MBE. Journal of Crystal Growth, 2001, 222, 685-691.	1.5	11
47	Linear scaling relaxation of the atomic positions in nanostructures. Physical Review B, 2001, 64, .	3.2	20
48	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
49	CO Oxidation on Pt(111): AnAb InitioDensity Functional Theory Study. Physical Review Letters, 1998, 80, 3650-3653.	7.8	675
50	Computer simulation of Au(001)/Ni multilayers: comparison with experiments. Journal of Physics Condensed Matter, 1995, 7, 6407-6421.	1.8	25
51	Quantitative analysis of the deformation and chemical profiles of strained multilayers. Ultramicroscopy, 1994, 56, 94-107.	1.9	60