FranÃ§ois Gygi

List of Publications by Year
in descending order

89	8,964	38738 50	48312 88
papers	citations	h-index	g-index

92	92	92	9187
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantum simulations of thermally activated delayed fluorescence in an all-organic emitter. Physical Chemistry Chemical Physics, 2022, 24, 10101-10113.	2.8	6
2	Free-Energy Landscape and Isomerization Rates of Au₄ Clusters at Finite Temperatures. Journal of Physical Chemistry A, 2022, 126, 3392-3400.	2.5	2
3	Code interoperability extends the scope of quantum simulations. Npj Computational Materials, 2021, 7, .	8.7	8
4	Neural Network Sampling of the Free Energy Landscape for Nitrogen Dissociation on Ruthenium. Journal of Physical Chemistry Letters, 2021, 12, 2954-2962.	4.6	16
5	Capturing the Complete Reaction Profile of a Câ€“H Bond Activation. Journal of the American Chemical Society, 2021, 143, 6060-6064.	13.7	21
6	Quantum vibronic effects on the electronic properties of solid and molecular carbon. Physical Review Materials, 2021, 5, .	2.4	12
7	Dissociation of salts in water under pressure. Nature Communications, 2020, 11, 3037.	12.8	21
8	Validating first-principles molecular dynamics calculations of oxide/water interfaces with x-ray reflectivity data. Physical Review Materials, 2020, 4, .	2.4	12
9	Finite-Field Approach to Solving the Bethe-Salpeter Equation. Physical Review Letters, 2019, 122, 237402.	7.8	35
10	Ensemble first-principles molecular dynamics simulations of water using the SCAN meta-GGA density functional. Journal of Chemical Physics, 2019, 151, 164101.	3.0	24
11	A Finite-Field Approach for GW Calculations beyond the Random Phase Approximation. Journal of Chemical Theory and Computation, 2019, 15, 154-164.	5.3	21
12	Hierarchical Coupling of First-Principles Molecular Dynamics with Advanced Sampling Methods. Journal of Chemical Theory and Computation, 2018, 14, 2881-2888.	5.3	18
13	Equilibration and analysis of first-principles molecular dynamics simulations of water. Journal of Chemical Physics, 2018, 148, 124501.	3.0	41
14	The role of defects and excess surface charges at finite temperature for optimizing oxide photoabsorbers. Nature Materials, 2018, 17, 1122-1127.	27.5	61
15	First-Principles Simulations of Liquid Water Using a Dielectric-Dependent Hybrid Functional. Journal of Physical Chemistry Letters, 2018, 9, 3068-3073.	4.6	82
16	First-principles simulations of heat transport. Physical Review Materials, 2017, 1, .	2.4	35
17	Blind test of density-functional-based methods on intermolecular interaction energies. Journal of Chemical Physics, 2016, 145, 124105.	3.0	97
18	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113

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19	Optimization algorithm for the generation of ONCV pseudopotentials. Computer Physics Communications, 2015, 196, 36-44.	7.5	805
20	Density and Compressibility of Liquid Water and Ice from First-Principles Simulations with Hybrid Functionals. Journal of Physical Chemistry Letters, 2015, 6, 2902-2908.	4.6	77
21	Performance and Accuracy of Recursive Subspace Bisection for Hybrid DFT Calculations in Inhomogeneous Systems. Journal of Chemical Theory and Computation, 2015, 11, 4655-4663.	5.3	28
22	Optimized Scheduling Strategies for Hybrid Density Functional theory Electronic Structure Calculations. , 2014, , .		2
23	Exotic phase Si nanoparticles and Si-ZnS nanocomposites: New paradigms to improve the efficiency of MEG solar cells. , 2014, , .		0
24	Electronic Structure of Aqueous Sulfuric Acid from First-Principles Simulations with Hybrid Functionals. Journal of Physical Chemistry Letters, 2014, 5, 2562-2567.	4.6	24
25	Solar Nanocomposites with Complementary Charge Extraction Pathways for Electrons and Holes: Si Embedded in ZnS. Physical Review Letters, 2014, 112, 106801.	7.8	22
26	Structural and electronic properties of aqueous NaCl solutions from ab initio molecular dynamics simulations with hybrid density functionals. Chemical Physics Letters, 2014, 604, 89-96.	2.6	74
27	Strongly Anisotropic Dielectric Relaxation of Water at the Nanoscale. Journal of Physical Chemistry Letters, 2013, 4, 2477-2481.	4.6	104
28	Raman Spectra of Liquid Water from Ab Initio Molecular Dynamics: Vibrational Signatures of Charge Fluctuations in the Hydrogen Bond Network. Journal of Chemical Theory and Computation, 2013, 9, 4124-4130.	5.3	74
29	Dimensionality and heat transport in Si-Ge superlattices. Applied Physics Letters, 2013, 102, .	3.3	47
30	Efficient Computation of Hartreeâ€“Fock Exchange Using Recursive Subspace Bisection. Journal of Chemical Theory and Computation, 2013, 9, 582-587.	5.3	53
31	Communication: Electronic structure of the solvated chloride anion from first principles molecular dynamics. Journal of Chemical Physics, 2013, 138, 181102.	3.0	46
32	Band offsets and dielectric properties of the amorphous Si3N4/Si(100) interface: A first-principles study. Applied Physics Letters, 2013, 102, .	3.3	23
33	Tungsten Oxide Clathrates for Water Oxidation: A First Principles Study. Chemistry of Materials, 2012, 24, 4252-4260.	6.7	37
34	A simplified implementation of van der Waals density functionals for first-principles molecular dynamics applications. Journal of Chemical Physics, 2012, 136, 224107.	3.0	49
35	A distributed approach to verification and validation of electronic structure simulation data using ESTEST. Computer Physics Communications, 2012, 183, 1744-1748.	7.5	2
36	Tailored Nanoheterojunctions for Optimized Light Emission. Physical Review Letters, 2011, 107, 206805.	7.8	22

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37	Structural and Vibrational Properties of Liquid Water from van der Waals Density Functionals. Journal of Chemical Theory and Computation, 2011, 7, 3054-3061.	5.3	146
38	First Principles Simulations of the Infrared Spectrum of Liquid Water Using Hybrid Density Functionals. Journal of Chemical Theory and Computation, 2011, 7, 1443-1449.	5.3	139
39	A scalable and accurate algorithm for the computation of Hartreeâ€“Fock exchange. Computer Physics Communications, 2010, 181, 855-860.	7.5	46
40	Optimizing Halley's Iteration for Computing the Matrix Polar Decomposition. SIAM Journal on Matrix Analysis and Applications, 2010, 31, 2700-2720.	1.4	42
41	Compact Representations of Kohn-Sham Invariant Subspaces. Physical Review Letters, 2009, 102, 166406.	7.8	51
42	Imperfect Crystal and Unusual Semiconductor: Boron, a Frustrated Element. Journal of the American Chemical Society, 2009, 131, 1903-1909.	13.7	114
43	Iterative calculations of dielectric eigenvalue spectra. Physical Review B, 2009, 79, .	3.2	86
44	Visual Analysis of Inter-Process Communication for Large-Scale Parallel Computing. IEEE Transactions on Visualization and Computer Graphics, 2009, 15, 1129-1136.	4.4	19
45	Practical algorithms to facilitate large-scale first-principles molecular dynamics. Journal of Physics: Conference Series, 2009, 180, 012074.	0.4	6
46	Electronic Structure of Thiolate-Covered Gold Nanoparticles: Au₁₀₂(MBA)₄₄. ACS Nano, 2008, 2, 1896-1902.	14.6	79
47	Water Confined in Nanotubes and between Graphene Sheets:â€‰ A First Principle Study. Journal of the American Chemical Society, 2008, 130, 1871-1878.	13.7	405
48	Dielectric Properties of Ice and Liquid Water from First-Principles Calculations. Physical Review Letters, 2008, 100, 147601.	7.8	63
49	Efficient iterative method for calculations of dielectric matrices. Physical Review B, 2008, 78, .	3.2	104
50	Melting of ice under pressure. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 14779-14783.	7.1	115
51	Surface Structure of CdSe Nanorods Revealed by Combined X-ray Absorption Fine Structure Measurements and ab Initio Calculations. Journal of Physical Chemistry C, 2007, 111, 75-79.	3.1	22
52	A First-Principles Molecular Dynamics Study of Calcium in Water. ChemPhysChem, 2005, 6, 1745-1749.	2.1	84
53	Linear scaling first-principles molecular dynamics with controlled accuracy. Computer Physics Communications, 2004, 162, 24-36.	7.5	55
54	Early chemistry in hot and dense nitromethane: Molecular dynamics simulations. Journal of Chemical Physics, 2004, 120, 10146-10153.	3.0	103

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55	Towards an assessment of the accuracy of density functional theory for first principles simulations of water. II. Journal of Chemical Physics, 2004, 121, 5400-5409.	3.0	338
56	Towards an assessment of the accuracy of density functional theory for first principles simulations of water. Journal of Chemical Physics, 2004, 120, 300-311.	3.0	489
57	A first principles simulation of rigid water. Journal of Chemical Physics, 2004, 120, 5192-5198.	3.0	77
58	Self-Healing of CdSe Nanocrystals: First-Principles Calculations. Physical Review Letters, 2004, 92, 217401.	7.8	214
59	Melting of Lithium Hydride under Pressure. Physical Review Letters, 2003, 91, 175502.	7.8	77
60	First-principles molecular dynamics simulations in a continuum solvent. International Journal of Quantum Chemistry, 2003, 93, 139-147.	2.0	125
61	Computation of Maximally Localized Wannier Functions usingÂaÂsimultaneous diagonalization algorithm. Computer Physics Communications, 2003, 155, 1-6.	7.5	86
62	Structure and Bonding of Dense Liquid Oxygen from First Principles Simulations. Physical Review Letters, 2003, 91, 265503.	7.8	26
63	Density functional theory for efficientab initio molecular dynamics simulations in solution. Journal of Computational Chemistry, 2002, 23, 662-666.	3.3	164
64	Dissociation of Water under Pressure. Physical Review Letters, 2001, 87, 265501.	7.8	174
65	Conformational dynamics of the dimethyl phosphate anion in solution. Chemical Physics Letters, 2001, 342, 434-440.	2.6	18
66	A first principles molecular dynamics simulation of the hydrated magnesium ion. Chemical Physics Letters, 2001, 343, 549-555.	2.6	164
67	Ab initiosimulations of compressed liquid deuterium. Physical Review B, 2000, 61, 909-912.	3.2	71
68	Water under Pressure. Physical Review Letters, 2000, 84, 2429-2432.	7.8	144
69	The solvation of Na+in water: First-principles simulations. Journal of Chemical Physics, 2000, 113, 4668-4673.	3.0	237
70	Quantum Mechanical Simulations of Microfracture in a Complex Material. Physical Review Letters, 1999, 82, 3476-3479.	7.8	24
71	Wetting Silicon Carbide with Nitrogen: A Theoretical Study. Physical Review Letters, 1999, 83, 2006-2009.	7.8	9
72	First-principles simulations of organic compounds: Solid CO2 under pressure. Computational Materials Science, 1998, 10, 63-66.	3.0	7

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73	Influence of stress and defects on the silicon-terminated SiC(001) surface structure. Physical Review B, 1998, 57, 12255-12261.	3.2	64
74	Vibrational and electronic properties of neutral and negatively chargedC20clusters. Physical Review B, 1998, 57, 1860-1867.	3.2	83
75	First-principles calculations of SiC(001) surface core level shifts. Applied Physics Letters, 1998, 72, 1902-1904.	3.3	21
76	Reconstruction and Thermal Stability of the Cubic SiC (001) Surfaces. Physical Review Letters, 1996, 77, 5090-5093.	7.8	77
77	Real-space adaptive-coordinate electronic-structure calculations. Physical Review B, 1995, 52, R2229-R2232.	3.2	201
78	Ab initiomolecular dynamics in adaptive coordinates. Physical Review B, 1995, 51, 11190-11193.	3.2	66
79	Ab initiostudy of positron trapping at a vacancy in GaAs. Physical Review Letters, 1994, 72, 3214-3217.	7.8	67
80	Reconstruction of the diamond (1 1 1) surface. Physica B: Condensed Matter, 1993, 185, 539-541.	2.7	1
81	Electronic-structure calculations in adaptive coordinates. Physical Review B, 1993, 48, 11692-11700.	3.2	193
82	Doping-induced distortions and bonding inK6C60andRb6C60. Physical Review Letters, 1992, 68, 823-826.	7.8	59
83	Reconstruction of the diamond (111) surface. Physical Review Letters, 1992, 69, 2947-2950.	7.8	113
84	Impurity states in doped fullerenes: C59B and C59N. Chemical Physics Letters, 1992, 190, 159-162.	2.6	171
85	Structural and electronic properties of C70. Chemical Physics Letters, 1992, 189, 241-244.	2.6	84
86	Self-consistent electronic structure of a vortex line in a type-II superconductor. Physical Review B, 1991, 43, 7609-7621.	3.2	358
87	Electronic tunneling into an isolated vortex in a clean type-II superconductor. Physical Review B, 1990, 41, 822-825.	3.2	97
88	Angular band structure of a vortex line in a type-II superconductor. Physical Review Letters, 1990, 65, 1820-1823.	7.8	59
89	Electron charge density of alkali halides beyond the rigid-ion approximation. Solid State Communications, 1984, 49, 437-439.	1.9	9