Franois Gygi

List of Publications by Year in Descending Order

86 papers	7,485 citations	48 h-index	86 g-index
92 ext. papers	8,259 ext. citations	6 avg, IF	6.1 L-index

#	Paper	IF	Citations
86	Capturing the Complete Reaction Profile of a C-H Bond Activation. *Journal of the American Chemical Society*, **2021**, 143, 6060-6064	16.4	7
85	Code interoperability extends the scope of quantum simulations. *Npj Computational Materials*, **2021**, 7,	10.9	2
84	Neural Network Sampling of the Free Energy Landscape for Nitrogen Dissociation on Ruthenium. *Journal of Physical Chemistry Letters*, **2021**, 12, 2954-2962	6.4	8
83	Quantum vibronic effects on the electronic properties of solid and molecular carbon. *Physical Review Materials*, **2021**, 5,	3.2	1
82	Dissociation of salts in water under pressure. *Nature Communications*, **2020**, 11, 3037	17.4	9
81	Validating first-principles molecular dynamics calculations of oxide/water interfaces with x-ray reflectivity data. *Physical Review Materials*, **2020**, 4,	3.2	5
80	Finite-Field Approach to Solving the Bethe-Salpeter Equation. *Physical Review Letters*, **2019**, 122, 237402	7.4	17
79	Ensemble first-principles molecular dynamics simulations of water using the SCAN meta-GGA density functional. *Journal of Chemical Physics*, **2019**, 151, 164101	3.9	17
78	A Finite-Field Approach for GW Calculations beyond the Random Phase Approximation. *Journal of Chemical Theory and Computation*, **2019**, 15, 154-164	6.4	15
77	Hierarchical Coupling of First-Principles Molecular Dynamics with Advanced Sampling Methods. *Journal of Chemical Theory and Computation*, **2018**, 14, 2881-2888	6.4	14
76	Equilibration and analysis of first-principles molecular dynamics simulations of water. *Journal of Chemical Physics*, **2018**, 148, 124501	3.9	34
75	The role of defects and excess surface charges at finite temperature for optimizing oxide photoabsorbers. *Nature Materials*, **2018**, 17, 1122-1127	27	48
74	First-Principles Simulations of Liquid Water Using a Dielectric-Dependent Hybrid Functional. *Journal of Physical Chemistry Letters*, **2018**, 9, 3068-3073	6.4	67
73	First-principles simulations of heat transport. *Physical Review Materials*, **2017**, 1,	3.2	25
72	Reproducibility in density functional theory calculations of solids. *Science*, **2016**, 351, aad3000	33.3	784
71	Blind test of density-functional-based methods on intermolecular interaction energies. *Journal of Chemical Physics*, **2016**, 145, 124105	3.9	76
70	Performance and accuracy of recursive subspace bisection for hybrid DFT calculations in inhomogeneous systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 4655-63	6.4	24

69	Optimization algorithm for the generation of ONCV pseudopotentials. *Computer Physics Communications*, **2015**, 196, 36-44	4.2	488
68	Density and Compressibility of Liquid Water and Ice from First-Principles Simulations with Hybrid Functionals. *Journal of Physical Chemistry Letters*, **2015**, 6, 2902-8	6.4	61
67	Electronic Structure of Aqueous Sulfuric Acid from First-Principles Simulations with Hybrid Functionals. *Journal of Physical Chemistry Letters*, **2014**, 5, 2562-7	6.4	20
66	Solar nanocomposites with complementary charge extraction pathways for electrons and holes: Si embedded in ZnS. *Physical Review Letters*, **2014**, 112, 106801	7.4	19
65	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	2.5	65
64	Optimized Scheduling Strategies for Hybrid Density Functional theory Electronic Structure Calculations **2014**,		1
63	Strongly Anisotropic Dielectric Relaxation of Water at the Nanoscale. *Journal of Physical Chemistry Letters*, **2013**, 4, 2477-2481	6.4	87
62	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, 4124-30	6.4	64
61	Dimensionality and heat transport in Si-Ge superlattices. *Applied Physics Letters*, **2013**, 102, 073113	3.4	41
60	Efficient Computation of Hartree-Fock Exchange Using Recursive Subspace Bisection. *Journal of Chemical Theory and Computation*, **2013**, 9, 582-7	6.4	42
59	Communication: electronic structure of the solvated chloride anion from first principles molecular dynamics. *Journal of Chemical Physics*, **2013**, 138, 181102	3.9	43
58	Band offsets and dielectric properties of the amorphous Si3N4/Si(100) interface: A first-principles study. *Applied Physics Letters*, **2013**, 102, 241603	3.4	19
57	A distributed approach to verification and validation of electronic structure simulation data using ESTEST. *Computer Physics Communications*, **2012**, 183, 1744-1748	4.2	2
56	Tungsten Oxide Clathrates for Water Oxidation: A First Principles Study. *Chemistry of Materials*, **2012**, 24, 4252-4260	9.6	31
55	A simplified implementation of van der Waals density functionals for first-principles molecular dynamics applications. *Journal of Chemical Physics*, **2012**, 136, 224107	3.9	39
54	Tailored nanoheterojunctions for optimized light emission. *Physical Review Letters*, **2011**, 107, 206805	7.4	19
53	Structural and Vibrational Properties of Liquid Water from van der Waals Density Functionals. *Journal of Chemical Theory and Computation*, **2011**, 7, 3054-61	6.4	134
52	First Principles Simulations of the Infrared Spectrum of Liquid Water Using Hybrid Density Functionals. *Journal of Chemical Theory and Computation*, **2011**, 7, 1443-9	6.4	127

51	Optimizing Halley's Iteration for Computing the Matrix Polar Decomposition. *SIAM Journal on Matrix Analysis and Applications*, **2010**, 31, 2700-2720	1.5	27
50	A scalable and accurate algorithm for the computation of Hartree–Fock exchange. *Computer Physics Communications*, **2010**, 181, 855-860	4.2	38
49	Compact representations of Kohn-Sham invariant subspaces. *Physical Review Letters*, **2009**, 102, 166406	7.4	44
48	Imperfect crystal and unusual semiconductor: boron, a frustrated element. *Journal of the American Chemical Society*, **2009**, 131, 1903-9	16.4	104
47	Iterative calculations of dielectric eigenvalue spectra. *Physical Review B*, **2009**, 79,	3.3	77
46	Visual analysis of inter-process communication for large-scale parallel computing. *IEEE Transactions on Visualization and Computer Graphics*, **2009**, 15, 1129-36	4	16
45	Practical algorithms to facilitate large-scale first-principles molecular dynamics. *Journal of Physics: Conference Series*, **2009**, 180, 012074	0.3	6
44	Electronic structure of thiolate-covered gold nanoparticles: Au102(MBA)44. *ACS Nano*, **2008**, 2, 1896-902	16.7	73
43	Water confined in nanotubes and between graphene sheets: a first principle study. *Journal of the American Chemical Society*, **2008**, 130, 1871-8	16.4	353
42	Dielectric properties of ice and liquid water from first-principles calculations. *Physical Review Letters*, **2008**, 100, 147601	7.4	59
41	Efficient iterative method for calculations of dielectric matrices. *Physical Review B*, **2008**, 78,	3.3	88
40	Melting of ice under pressure. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 14779-83	11.5	107
39	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	3.8	19
38	A first-principles molecular dynamics study of calcium in water. *ChemPhysChem*, **2005**, 6, 1745-9	3.2	77
37	Linear scaling first-principles molecular dynamics with controlled accuracy. *Computer Physics Communications*, **2004**, 162, 24-36	4.2	52
36	Early chemistry in hot and dense nitromethane: molecular dynamics simulations. *Journal of Chemical Physics*, **2004**, 120, 10146-53	3.9	94
35	Towards an assessment of the accuracy of density functional theory for first principles simulations of water. II. *Journal of Chemical Physics*, **2004**, 121, 5400-9	3.9	326
34	Towards an assessment of the accuracy of density functional theory for first principles simulations of water. *Journal of Chemical Physics*, **2004**, 120, 300-11	3.9	458

33	A first principles simulation of rigid water. *Journal of Chemical Physics*, **2004**, 120, 5192-8	3.9	73
32	Self-healing of CdSe nanocrystals: first-principles calculations. *Physical Review Letters*, **2004**, 92, 217401	7.4	200
31	Melting of lithium hydride under pressure. *Physical Review Letters*, **2003**, 91, 175502	7.4	68
30	First-principles molecular dynamics simulations in a continuum solvent. *International Journal of Quantum Chemistry*, **2003**, 93, 139-147	2.1	112
29	Computation of Maximally Localized Wannier Functions using a simultaneous diagonalization algorithm. *Computer Physics Communications*, **2003**, 155, 1-6	4.2	68
28	Structure and bonding of dense liquid oxygen from first principles simulations. *Physical Review Letters*, **2003**, 91, 265503	7.4	24
27	Density functional theory for efficient ab initio molecular dynamics simulations in solution. *Journal of Computational Chemistry*, **2002**, 23, 662-6	3.5	145
26	Conformational dynamics of the dimethyl phosphate anion in solution. *Chemical Physics Letters*, **2001**, 342, 434-440	2.5	17
25	A first principles molecular dynamics simulation of the hydrated magnesium ion. *Chemical Physics Letters*, **2001**, 343, 549-555	2.5	152
24	Dissociation of water under pressure. *Physical Review Letters*, **2001**, 87, 265501	7.4	144
23	Ab initio simulations of compressed liquid deuterium. *Physical Review B*, **2000**, 61, 909-912	3.3	71
22	Water under pressure. *Physical Review Letters*, **2000**, 84, 2429-32	7.4	135
21	The solvation of Na+ in water: First-principles simulations. *Journal of Chemical Physics*, **2000**, 113, 4668-4673	3.9	220
20	Quantum Mechanical Simulations of Microfracture in a Complex Material. *Physical Review Letters*, **1999**, 82, 3476-3479	7.4	21
19	Wetting Silicon Carbide with Nitrogen: A Theoretical Study. *Physical Review Letters*, **1999**, 83, 2006-2009	7.4	8
18	First-principles simulations of organic compounds: Solid CO2 under pressure. *Computational Materials Science*, **1998**, 10, 63-66	3.2	6
17	Influence of stress and defects on the silicon-terminated SiC(001) surface structure. *Physical Review B*, **1998**, 57, 12255-12261	3.3	60
16	Vibrational and electronic properties of neutral and negatively charged C20 clusters. *Physical Review B*, **1998**, 57, 1860-1867	3.3	79

15	First-principles calculations of SiC(001) surface core level shifts. *Applied Physics Letters*, **1998**, 72, 1902-1904	3.4	18
14	Reconstruction and Thermal Stability of the Cubic SiC (001) Surfaces. *Physical Review Letters*, **1996**, 77, 5090-5093	7.4	73
13	Real-space adaptive-coordinate electronic-structure calculations. *Physical Review B*, **1995**, 52, R2229-R2232	3.3	168
12	Ab initio molecular dynamics in adaptive coordinates. *Physical Review B*, **1995**, 51, 11190-11193	3.3	59
11	Ab initio study of positron trapping at a vacancy in GaAs. *Physical Review Letters*, **1994**, 72, 3214-3217	7.4	64
10	Electronic-structure calculations in adaptive coordinates. *Physical Review B*, **1993**, 48, 11692-11700	3.3	163
9	Reconstruction of the diamond (1 1 1) surface. *Physica B: Condensed Matter*, **1993**, 185, 539-541	2.8	1
8	Doping-induced distortions and bonding in K6C60 and Rb6C60. *Physical Review Letters*, **1992**, 68, 823-826	7.4	57
7	Reconstruction of the diamond (111) surface. *Physical Review Letters*, **1992**, 69, 2947-2950	7.4	111
6	Impurity states in doped fullerenes: C59B and C59N. *Chemical Physics Letters*, **1992**, 190, 159-162	2.5	155
5	Structural and electronic properties of C70. *Chemical Physics Letters*, **1992**, 189, 241-244	2.5	75
4	Self-consistent electronic structure of a vortex line in a type-II superconductor. *Physical Review B*, **1991**, 43, 7609-7621	3.3	308
3	Electronic tunneling into an isolated vortex in a clean type-II superconductor. *Physical Review B*, **1990**, 41, 822-825	3.3	91
2	Angular band structure of a vortex line in a type-II superconductor. *Physical Review Letters*, **1990**, 65, 1820-1823	7.4	55
1	Electron charge density of alkali halides beyond the rigid-ion approximation. *Solid State Communications*, **1984**, 49, 437-439	1.6	7