

Henry Krakauer

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

80 papers	4,276 citations	34 h-index	65 g-index
82 ext. papers	4,499 ext. citations	4.3 avg, IF	5.23 L-index

#	Paper	IF	Citations
80	Ab initio calculations in atoms, molecules, and solids, treating spin-orbit coupling and electron interaction on an equal footing.. <i>Journal of Chemical Physics</i> , 2022 , 156, 014107	3.9	1
79	Local Embedding and Effective Downfolding in the Auxiliary-Field Quantum Monte Carlo Method. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 3949-3959	6.4	6
78	Auxiliary-field quantum Monte Carlo calculations with multiple-projector pseudopotentials. <i>Physical Review B</i> , 2017 , 95,	3.3	16
77	Auxiliary-field quantum Monte Carlo calculations of the molybdenum dimer. <i>Journal of Chemical Physics</i> , 2016 , 144, 244306	3.9	9
76	An auxiliary-field quantum Monte Carlo study of the chromium dimer. <i>Journal of Chemical Physics</i> , 2015 , 142, 064302	3.9	44
75	Electron-phonon coupling and exchange-correlation effects in superconducting H3S under high pressure. <i>Physical Review B</i> , 2015 , 92,	3.3	28
74	Quantum Monte Carlo Calculations in Solids with Downfolded Hamiltonians. <i>Physical Review Letters</i> , 2015 , 114, 226401	7.4	40
73	Stability, energetics, and magnetic states of cobalt adatoms on graphene. <i>Physical Review Letters</i> , 2014 , 113, 175502	7.4	38
72	Electronic Structure and Total Energy Calculations for Oxide Perovskites and Superconductors. <i>Geophysical Monograph Series</i> , 2013 , 55-66	1.1	8
71	Frozen-Orbital and Downfolding Calculations with Auxiliary-Field Quantum Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 4825-33	6.4	26
70	Excited state calculations in solids by auxiliary-field quantum Monte Carlo. <i>New Journal of Physics</i> , 2013 , 15, 093017	2.9	33
69	Ab initio many-body study of cobalt adatoms adsorbed on graphene. <i>Physical Review B</i> , 2012 , 86,	3.3	23
68	First-principles calculations of ^{17}O nuclear magnetic resonance chemical shielding in $\text{Pb}(\text{Zr}(1/2)\text{Ti}(1/2))\text{O}_3$ and $\text{Pb}(\text{Mg}(1/3)\text{Nb}(2/3))\text{O}_3$: linear dependence on transition-metal/oxygen bond lengths. <i>Journal of Chemical Physics</i> , 2011 , 135, 114507	3.9	5
67	Finite-size correction in many-body electronic structure calculations of magnetic systems. <i>Physical Review B</i> , 2011 , 84,	3.3	14
66	Assessing weak hydrogen binding on Ca^+ centers: an accurate many-body study with large basis sets. <i>Journal of Chemical Physics</i> , 2011 , 135, 164105	3.9	41
65	High sensitivity of ^{17}O NMR to p-d hybridization in transition metal perovskites: first principles calculations of large anisotropic chemical shielding. <i>Journal of Chemical Physics</i> , 2009 , 131, 184511	3.9	4
64	Pressure-induced diamond to β -tin transition in bulk silicon: A quantum Monte Carlo study. <i>Physical Review B</i> , 2009 , 80,	3.3	50

63	Excited state calculations using phaseless auxiliary-field quantum Monte Carlo: Potential energy curves of low-lying C(2) singlet states. <i>Journal of Chemical Physics</i> , 2009 , 130, 094107	3.9	54
62	Stereochemistry determination by powder X-ray diffraction analysis and NMR spectroscopy residual dipolar couplings. <i>Angewandte Chemie - International Edition</i> , 2009 , 48, 5670-4	16.4	49
61	Eliminating spin contamination in auxiliary-field quantum Monte Carlo: realistic potential energy curve of F(2). <i>Journal of Chemical Physics</i> , 2008 , 128, 114309	3.9	47
60	Finite-size correction in many-body electronic structure calculations. <i>Physical Review Letters</i> , 2008 , 100, 126404	7.4	93
59	A study of H+H ₂ and several H-bonded molecules by phaseless auxiliary-field quantum Monte Carlo with plane wave and Gaussian basis sets. <i>Journal of Chemical Physics</i> , 2007 , 126, 194105	3.9	17
58	Bond breaking with auxiliary-field quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2007 , 127, 144101	3.9	40
57	Phaseless auxiliary-field quantum Monte Carlo calculations with plane waves and pseudopotentials: Applications to atoms and molecules. <i>Physical Review B</i> , 2007 , 75,	3.3	55
56	Structural dependence of electric field gradients in Pb(Zr _{1-x} Ti _x)O ₃ from first principles. <i>Physical Review B</i> , 2007 , 76,	3.3	11
55	Auxiliary-field quantum Monte Carlo study of first- and second-row post-d elements. <i>Journal of Chemical Physics</i> , 2006 , 125, 154110	3.9	22
54	Auxiliary-field quantum Monte Carlo study of TiO and MnO molecules. <i>Physical Review B</i> , 2006 , 73,	3.3	34
53	Wannier functions and Born charge tensors of brookite TiO ₂ . <i>Physical Review B</i> , 2006 , 74,	3.3	18
52	Auxiliary-field quantum Monte Carlo calculations of molecular systems with a Gaussian basis. <i>Journal of Chemical Physics</i> , 2006 , 124, 224101	3.9	69
51	Quantum simulations of realistic systems by auxiliary fields. <i>Computer Physics Communications</i> , 2005 , 169, 394-399	4.2	16
50	Kinetic Monte Carlo simulations of crystal growth in ferroelectric alloys. <i>Physical Review B</i> , 2005 , 71,	3.3	2
49	Born charge differences of TiO ₂ polytypes: Multipole expansion of Wannier charge densities. <i>Physical Review B</i> , 2004 , 69,	3.3	26
48	Quantum Monte Carlo method using phase-free random walks with Slater determinants. <i>Physical Review Letters</i> , 2003 , 90, 136401	7.4	213
47	First-principles calculations of piezoelectricity and polarization rotation in Pb(Zr _{0.5} Ti _{0.5})O ₃ . <i>Physical Review B</i> , 2003 , 68,	3.3	64
46	Charge-transfer electrostatic model of compositional order in perovskite alloys. <i>Physical Review B</i> , 2001 , 63,	3.3	13

45	Dynamic local distortions in KNbO ₃ . <i>Journal of Physics Condensed Matter</i> , 1999 , 11, 3779-3787	1.8	38
44	Precursor structures in ferroelectrics from first-principles calculations. <i>Ferroelectrics</i> , 1998 , 206, 133-155.	0.6	19
43	Effective Hamiltonian for the ferroelectric phase transitions in KNbO ₃ 1998 ,		2
42	First-principles study of SrTiO ₃ in cubic and tetragonal phases 1998 ,		1
41	Ab initio linear response study of SrTiO ₃ . <i>Ferroelectrics</i> , 1997 , 194, 109-118	0.6	78
40	Born effective charges, dielectric constants, and lattice dynamics of KNbO ₃ . <i>Ferroelectrics</i> , 1997 , 194, 97-107	0.6	5
39	Polarization dependence of Born effective charge and dielectric constant in KNbO ₃ . <i>Physical Review B</i> , 1996 , 54, 11161-11168	3.3	51
38	Wavevector dependence of ferroelectric instabilities in KNbO ₃ . <i>Journal of Physics and Chemistry of Solids</i> , 1996 , 57, 1409-1412	3.9	4
37	Pressure dependence of Born effective charges, dielectric constant, and lattice dynamics in SiC. <i>Physical Review B</i> , 1996 , 53, 5430-5437	3.3	42
36	Ab initio linear response calculations of lattice dynamics using an LAPW basis. <i>International Journal of Quantum Chemistry</i> , 1995 , 56, 131-136	2.1	
35	Lattice dynamics of ferroelectrics using the lapw linear response method: Application to KNbO ₃ . <i>Ferroelectrics</i> , 1995 , 164, 161-167	0.6	9
34	First-Principles Determination of Chain-Structure Instability in KNbO ₃ . <i>Physical Review Letters</i> , 1995 , 74, 4067-4070	7.4	143
33	Linearized-augmented-plane-wave method with Car-Parrinello scaling. <i>Physical Review B</i> , 1994 , 49, 17424-17427	3.3	33
32	Ab initio lapw linear response method for ferroelectrics. <i>Ferroelectrics</i> , 1994 , 151, 39-47	0.6	
31	Theoretical determination that electrons act as anions in the electride Cs ⁺ (15-crown-5)2Li ⁻ . <i>Nature</i> , 1993 , 365, 39-42	50.4	87
30	Linear response calculations using lapw and mixed basis methods. <i>Ferroelectrics</i> , 1992 , 136, 105-112	0.6	2
29	Electronic structure studies of the differences in ferroelectric behavior of BaTiO ₃ and PbTiO ₃ . <i>Ferroelectrics</i> , 1992 , 136, 65-83	0.6	308
28	Electronic structure and electron-phonon coupling in layered copper oxide superconductors. <i>Physica B: Condensed Matter</i> , 1991 , 169, 45-50	2.8	12

27	Evidence of strong electron-phonon coupling in the high T _c copper oxide superconductors. <i>International Journal of Quantum Chemistry</i> , 1990 , 38, 693-699	2.1	2
26	Martensitic transformation of Ca. <i>Physical Review B</i> , 1990 , 42, 4563-4567	3.3	21
25	First principles calculations for ferroelectrics in vision. <i>Ferroelectrics</i> , 1990 , 111, 1-7	0.6	6
24	Positron annihilation in high-T _c superconductors. <i>Physical Review B</i> , 1989 , 39, 9667-9670	3.3	58
23	Ground-state properties of fcc and bcc lanthanum. <i>Physical Review B</i> , 1989 , 39, 4921-4925	3.3	21
22	Total-energy study of the equation of state of HgTe and HgSe. <i>Physical Review B</i> , 1989 , 39, 10154-10161	3.3	31
21	Electronic structure and bonding of the Cu/W(001) surface alloy. <i>Surface Science</i> , 1989 , 216, 303-310	1.8	29
20	Analysis of electronic structure and charge density of the high-temperature superconductor YBa ₂ Cu ₃ O ₇ . <i>Journal of Superconductivity and Novel Magnetism</i> , 1988 , 1, 111-141		192
19	Effect of bismuth on high-T _c cuprate superconductors: Electronic structure of Bi ₂ Sr. <i>Physical Review Letters</i> , 1988 , 60, 1665-1667	7.4	314
18	Bonding and reconstruction of the W(001) surface. <i>Physical Review B</i> , 1988 , 37, 3999-4006	3.3	73
17	Anisotropic normal-state transport properties predicted and analyzed for high-T _c oxide superconductors. <i>Physical Review B</i> , 1988 , 37, 7482-7490	3.3	357
16	Local-density-approximation study of LaS and SmS. <i>Physical Review B</i> , 1988 , 37, 10045-10049	3.3	25
15	Smooth Fourier interpolation of periodic functions. <i>Physical Review B</i> , 1988 , 38, 2721-2726	3.3	72
14	Local-density description of antiferromagnetic Cr. <i>Physical Review B</i> , 1988 , 38, 12834-12836	3.3	33
13	First-Principles Phonon Calculations for La ₂ CuO ₄ . <i>Materials Research Society Symposia Proceedings</i> , 1988 , 141, 171		
12	Band-theory analysis of anisotropic transport in La ₂ CuO. <i>Physical Review B</i> , 1987 , 36, 3926-3929	3.3	150
11	Equilibrium properties of hcp titanium and zirconium. <i>Physical Review B</i> , 1987 , 36, 7335-7341	3.3	41
10	Anisotropic Normal State Transport Properties of Oxide Superconductors Predicted from Lapw Band Structures. <i>Materials Research Society Symposia Proceedings</i> , 1987 , 99, 183		

9	Lattice Dynamics and Ionicity in the High-Temperature Superconductors. <i>Materials Research Society Symposia Proceedings</i> , 1987 , 99, 825		2
8	The solution of large dense generalized eigenvalue problems on the cray X-MP/24 with SSD. <i>Journal of Computational Physics</i> , 1987 , 69, 471-481	4.1	10
7	Linearized Augmented Plane Wave (LAPW) Method for Isolated Clusters and Molecules 1987 , 517-521		
6	Prediction of Anisotropic Thermopower of $\text{La}_{2-x}\text{M}_x\text{CuO}_4$ 1987 , 489-491		4
5	Accelerating the convergence of self-consistent linearized augmented-plane-wave calculations. <i>Physical Review B</i> , 1986 , 34, 8391-8393	3.3	96
4	Instability of the ideal tungsten (001) surface. <i>Physical Review Letters</i> , 1986 , 57, 3292-3295	7.4	58
3	Local-density-functional calculation of the pressure-induced metallization of BaSe and BaTe. <i>Physical Review Letters</i> , 1985 , 55, 1200-1203	7.4	476
2	Linearized augmented-plane-wave calculation of the electronic structure and total energy of tungsten. <i>Physical Review B</i> , 1985 , 32, 7792-7797	3.3	132
1	Method for calculating surface electronic structure of noble and transition metals. <i>Physical Review B</i> , 1977 , 16, 605-616	3.3	33