Henry Krakauer

List of Publications by Citations

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	Local-density-functional calculation of the pressure-induced metallization of BaSe and BaTe. *Physical Review Letters*, **1985**, 55, 1200-1203	7.4	476
79	Anisotropic normal-state transport properties predicted and analyzed for high-Tc oxide superconductors. *Physical Review B*, **1988**, 37, 7482-7490	3.3	357
78	Effect of bismuth on high-Tc cuprate superconductors: Electronic structure of Bi2Sr. *Physical Review Letters*, **1988**, 60, 1665-1667	7.4	314
77	Electronic structure studies of the differences in ferroelectric behavior of batio3 and PbTiO3. *Ferroelectrics*, **1992**, 136, 65-83	0.6	308
76	Quantum Monte Carlo method using phase-free random walks with slater determinants. *Physical Review Letters*, **2003**, 90, 136401	7.4	213
75	Analysis of electronic structure and charge density of the high-temperature superconductor YBa2Cu3O7. *Journal of Superconductivity and Novel Magnetism*, **1988**, 1, 111-141		192
74	Band-theory analysis of anisotropic transport in La2CuO. *Physical Review B*, **1987**, 36, 3926-3929	3.3	150
73	First-Principles Determination of Chain-Structure Instability in KNbO3. *Physical Review Letters*, **1995**, 74, 4067-4070	7.4	143
72	Linearized augmented-plane-wave calculation of the electronic structure and total energy of tungsten. *Physical Review B*, **1985**, 32, 7792-7797	3.3	132
71	Accelerating the convergence of self-consistent linearized augmented-plane-wave calculations. *Physical Review B*, **1986**, 34, 8391-8393	3.3	96
70	Finite-size correction in many-body electronic structure calculations. *Physical Review Letters*, **2008**, 100, 126404	7.4	93
69	Theoretical determination that electrons act as anions in the electride Cs+ (15-crown-5)2e-. *Nature*, **1993**, 365, 39-42	50.4	87
68	Ab initio linear response study of SrTiO3. *Ferroelectrics*, **1997**, 194, 109-118	0.6	78
67	Bonding and reconstruction of the W(001) surface. *Physical Review B*, **1988**, 37, 3999-4006	3.3	73
66	Smooth Fourier interpolation of periodic functions. *Physical Review B*, **1988**, 38, 2721-2726	3.3	72
65	Auxiliary-field quantum Monte Carlo calculations of molecular systems with a Gaussian basis. *Journal of Chemical Physics*, **2006**, 124, 224101	3.9	69
64	First-principles calculations of piezoelectricity and polarization rotation in Pb(Zr0.5Ti0.5)O3. *Physical Review B*, **2003**, 68,	3.3	64

63	Positron annihilation in high-Tc superconductors. *Physical Review B*, **1989**, 39, 9667-9670	3.3	58
62	Instability of the ideal tungsten (001) surface. *Physical Review Letters*, **1986**, 57, 3292-3295	7.4	58
61	Phaseless auxiliary-field quantum Monte Carlo calculations with plane waves and pseudopotentials: Applications to atoms and molecules. *Physical Review B*, **2007**, 75,	3.3	55
60	Excited state calculations using phaseless auxiliary-field quantum Monte Carlo: Potential energy curves of low-lying C(2) singlet states. *Journal of Chemical Physics*, **2009**, 130, 094107	3.9	54
59	Polarization dependence of Born effective charge and dielectric constant in KNbO3. *Physical Review B*, **1996**, 54, 11161-11168	3.3	51
58	Pressure-induced diamond to Etin transition in bulk silicon: A quantum Monte Carlo study. *Physical Review B*, **2009**, 80,	3.3	50
57	Stereochemistry determination by powder X-ray diffraction analysis and NMR spectroscopy residual dipolar couplings. *Angewandte Chemie - International Edition*, **2009**, 48, 5670-4	16.4	49
56	Eliminating spin contamination in auxiliary-field quantum Monte Carlo: realistic potential energy curve of F(2). *Journal of Chemical Physics*, **2008**, 128, 114309	3.9	47
55	An auxiliary-field quantum Monte Carlo study of the chromium dimer. *Journal of Chemical Physics*, **2015**, 142, 064302	3.9	44
54	Pressure dependence of Born effective charges, dielectric constant, and lattice dynamics in SiC. *Physical Review B*, **1996**, 53, 5430-5437	3.3	42
53	Assessing weak hydrogen binding on Ca+ centers: an accurate many-body study with large basis sets. *Journal of Chemical Physics*, **2011**, 135, 164105	3.9	41
52	Equilibrium properties of hcp titanium and zirconium. *Physical Review B*, **1987**, 36, 7335-7341	3.3	41
51	Quantum Monte Carlo Calculations in Solids with Downfolded Hamiltonians. *Physical Review Letters* , **2015**, 114, 226401	7.4	40
50	Bond breaking with auxiliary-field quantum Monte Carlo. *Journal of Chemical Physics*, **2007**, 127, 144101	3.9	40
49	Stability, energetics, and magnetic states of cobalt adatoms on graphene. *Physical Review Letters*, **2014**, 113, 175502	7.4	38
48	Dynamic local distortions in KNbO3. *Journal of Physics Condensed Matter*, **1999**, 11, 3779-3787	1.8	38
47	Auxiliary-field quantum Monte Carlo study of TiO and MnO molecules. *Physical Review B*, **2006**, 73,	3.3	34
46	Excited state calculations in solids by auxiliary-field quantum Monte Carlo. *New Journal of Physics*, **2013**, 15, 093017	2.9	33

45	Local-density description of antiferromagnetic Cr. *Physical Review B*, **1988**, 38, 12834-12836	3.3	33
44	Method for calculating surface electronic structure of noble and transition metals. *Physical Review B*, **1977**, 16, 605-616	3.3	33
43	Total-energy study of the equation of state of HgTe and HgSe. *Physical Review B*, **1989**, 39, 10154-10161	3.3	31
42	Electronic structure and bonding of the Cu/W(001) surface alloy. *Surface Science*, **1989**, 216, 303-310	1.8	29
41	Electron-phonon coupling and exchange-correlation effects in superconducting H3S under high pressure. *Physical Review B*, **2015**, 92,	3.3	28
40	Frozen-Orbital and Downfolding Calculations with Auxiliary-Field Quantum Monte Carlo. *Journal of Chemical Theory and Computation*, **2013**, 9, 4825-33	6.4	26
39	Born charge differences of TiO2 polytypes: Multipole expansion of Wannier charge densities. *Physical Review B*, **2004**, 69,	3.3	26
38	Local-density-approximation study of LaS and SmS. *Physical Review B*, **1988**, 37, 10045-10049	3.3	25
37	Ab initio many-body study of cobalt adatoms adsorbed on graphene. *Physical Review B*, **2012**, 86,	3.3	23
36	Auxiliary-field quantum Monte Carlo study of first- and second-row post-d elements. *Journal of Chemical Physics*, **2006**, 125, 154110	3.9	22
35	Ground-state properties of fcc and bcc lanthanum. *Physical Review B*, **1989**, 39, 4921-4925	3.3	21
34	Martensitic transformation of Ca. *Physical Review B*, **1990**, 42, 4563-4567	3.3	21
33	Precursor structures in ferroelectrics from first-principles calculations. *Ferroelectrics*, **1998**, 206, 133-155	0.6	19
32	Wannier functions and Born charge tensors of brookite TiO2. *Physical Review B*, **2006**, 74,	3.3	18
31	A study of H+H2 and several H-bonded molecules by phaseless auxiliary-field quantum Monte Carlo with plane wave and Gaussian basis sets. *Journal of Chemical Physics*, **2007**, 126, 194105	3.9	17
30	Auxiliary-field quantum Monte Carlo calculations with multiple-projector pseudopotentials. *Physical Review B*, **2017**, 95,	3.3	16
29	Quantum simulations of realistic systems by auxiliary fields. *Computer Physics Communications*, **2005**, 169, 394-399	4.2	16
28	Finite-size correction in many-body electronic structure calculations of magnetic systems. *Physical Review B*, **2011**, 84,	3.3	14

27	Charge-transfer electrostatic model of compositional order in perovskite alloys. *Physical Review B*, **2001**, 63,	3.3	13
26	Electronic structure and electron-phonon coupling in layered copper oxide superconductors. *Physica B: Condensed Matter*, **1991**, 169, 45-50	2.8	12
25	Structural dependence of electric field gradients in Pb(Zr1−xTix)O3 from first principles. *Physical Review B*, **2007**, 76,	3.3	11
24	The solution of large dense generalized eigenvalue problems on the cray X-MP/24 with SSD. *Journal of Computational Physics*, **1987**, 69, 471-481	4.1	10
23	Lattice dynamics of ferroelectrics using the lapw linear response method: Application to KNbO3. *Ferroelectrics*, **1995**, 164, 161-167	0.6	9
22	Auxiliary-field quantum Monte Carlo calculations of the molybdenum dimer. *Journal of Chemical Physics*, **2016**, 144, 244306	3.9	9
21	Electronic Structure and Total Energy Calculations for Oxide Perovskites and Superconductors. *Geophysical Monograph Series*, **2013**, 55-66	1.1	8
20	Local Embedding and Effective Downfolding in the Auxiliary-Field Quantum Monte Carlo Method. *Journal of Chemical Theory and Computation*, **2019**, 15, 3949-3959	6.4	6
19	First principles calculations for ferroelectrics a vision. *Ferroelectrics*, **1990**, 111, 1-7	0.6	6
18	First-principles calculations of 17O nuclear magnetic resonance chemical shielding in Pb(Zr(1/2)Ti(1/2))O3 and Pb(Mg(1/3)Nb(2/3))O3: linear dependence on transition-metal/oxygen bond lengths. *Journal of Chemical Physics*, **2011**, 135, 114507	3.9	5
17	Born effective charges, dielectric constants, and lattice dynamics of KNbO3. *Ferroelectrics*, **1997**, 194, 97-107	0.6	5
16	High sensitivity of 17O NMR to p-d hybridization in transition metal perovskites: first principles calculations of large anisotropic chemical shielding. *Journal of Chemical Physics*, **2009**, 131, 184511	3.9	4
15	Wavevector dependence of ferroelectric instabilities in KNbO3. *Journal of Physics and Chemistry of Solids*, **1996**, 57, 1409-1412	3.9	4
14	Prediction of Anisotropic Thermopower of La2−MxCuO4 **1987**, 489-491		4
13	Linearized-augmented-plane-wave method with Car-Parrinello scaling. *Physical Review B*, **1994**, 49, 17424-17427	3.3	3
12	Kinetic Monte Carlo simulations of crystal growth in ferroelectric alloys. *Physical Review B*, **2005**, 71,	3.3	2
11	Effective Hamiltonian for the ferroelectric phase transitions in KNbO3 **1998**,		2
10	Linear response calculations using lapw and mixed basis methods. *Ferroelectrics*, **1992**, 136, 105-112	0.6	2

9	Evidence of strong electron–phonon coupling in the high Tc copper oxide superconductors. *International Journal of Quantum Chemistry*, **1990**, 38, 693-699	2.1	2
8	Lattice Dynamics and Ionicity in the High-Temperature Superconductors. *Materials Research Society Symposia Proceedings*, **1987**, 99, 825		2
7	First-principles study of SrTiO3 in cubic and tetragonal phases **1998**,		1
6	Ab initio calculations in atoms, molecules, and solids, treating spin-orbit coupling and electron interaction on an equal footing.. *Journal of Chemical Physics*, **2022**, 156, 014107	3.9	1
5	Ab initio linear response calculations of lattice dynamics using an LAPW basis. *International Journal of Quantum Chemistry*, **1995**, 56, 131-136	2.1	
4	Ab initio lapw linear response method for ferroelectrics. *Ferroelectrics*, **1994**, 151, 39-47	0.6	
3	Anisotropic Normal State Transport Properties of Oxide Superconductors Predicted from Lapw Band Structures. *Materials Research Society Symposia Proceedings*, **1987**, 99, 183		
2	First-Principles Phonon Calculations for LA2CUO4. *Materials Research Society Symposia Proceedings*, **1988**, 141, 171		
1	Linearized Augmented Plane Wave (LAPW) Method for Isolated Clusters and Molecules **1987**, 517-521		