N A W Holzwarth

List of Publications by Year
in descending order

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55	2,713	218677	175258
papers	citations	26 h-index	52 g-index

58	58	58	2320
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Cubic spline solver for generalized density functional treatments of atoms and generation of atomic datasets for use with exchange-correlation functionals including meta-GGA. Physical Review B, 2022, 105, .	3.2	9
2	Computational study of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Li</mml:mi><mml:mn>3</mml:mn></mml:m and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Li</mml:mi><mml:mn>3</mml:mn></mml:m I: Electrolyte properties of pure and doped crystals. Physical Review Materials, 2021, 5, .	2.4	3
3	Computational Investigation of the Electrolyte Properties of Li₁₂P₃N₉ and Its High Pressure Polymorph Li₄PN₃ through First-Principles Simulations. Journal of the Electrochemical Society, 2020, 167, 060505.	2.9	2
4	Li₄SnS₄and Li₄SnSe₄: Simulations of Their Structure and Electrolyte Properties. Journal of the Electrochemical Society, 2017, 164, A6386-A6394.	2.9	10
5	Unraveling the electrolyte properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Na</mml:mi><mml:mn>3</mml:mn></mml: through computation and experiment. Physical Review Materials, 2017, 1, .	2.4	21
6	First-principles simulations of the porous layered calcogenides<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Li</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Li</mml:mi><mml:mrow><mml:mn>2</mml Physical Review B, 2016, 94, .	3.2	12
7	Computational Study of Li Ion Electrolytes Composed of Li₃AsS₄Alloyed with Li₄GeS₄. Journal of the Electrochemical Society, 2016, 163, A2079-A2088.	2.9	10
8	Crystalline Inorganic Solid Electrolytes: Computer Simulations and Comparisons with Experiment. Materials and Energy, 2015, , 191-232.	0.1	1
9	Fast Lithium Ion Conduction in Li₂SnS₃: Synthesis, Physicochemical Characterization, and Electronic Structure. Chemistry of Materials, 2015, 27, 189-196.	6.7	85
10	Cu2ZnSnSxO4â^'x and Cu2ZnSnSxSe4â^'x: First principles simulations of optimal alloy configurations and their energies. Journal of Applied Physics, 2014, 115, .	2.5	22
11	Structures, <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mrow /><mml:mo>+</mml:mo></mml:msup></mml:math>mobilities, and interfacial properties of solid electrolytes Li<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>PS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow />	3.2	138
12	Computer Modeling of Crystalline Electrolytes: Lithium Thiophosphates and Phosphates. Journal of the Electrochemical Society, 2012, 159, A538-A547.	2.9	41
13	Adaptation of the projector-augmented-wave formalism to the treatment of orbital-dependent exchange-correlation functionals. Physical Review B, 2011, 84, .	3.2	1
14	Projector augmented wave formulation of Hartree-Fock calculations of electronic structure. Physical Review B, 2010, 81, .	3.2	3
15	First-principles study of LiPON and related solid electrolytes. Physical Review B, 2010, 81, .	3.2	47
16	Effects of O vacancies and N or Si substitutions on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mrow><mml:mtext>Li</mml:mtext></mml:mrow><mml:mo>+</mml:mo></mml:msup in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Li</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub> Physical Review B, 2008, 78, .	3.2	22
17	Li Ion Diffusion Mechanisms in the Crystalline Electrolyte Î³-Li[sub 3]PO[sub 4]. Journal of the Electrochemical Society, 2007, 154, A999.	2.9	66
18	Mechanisms of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mi mathvariant="normal">Li</mml:mi><mml:mo>+</mml:mo></mml:msup></mml:math>diffusion in crystalline<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î³</mml:mi></mml:math>- and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î²</mml:mi><mml:mi><</mml:mi>	3.2	93

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19	Method for calculating electronic structures near surfaces of semi-infinite crystals. Physical Review B, 2006, 73, .	3.2	3
20	Electronic structure of oxygen-related defects inPbWO4andCaMoO4crystals. Physical Review B, 2001, 64, .	3.2	64
21	Electronic band structures of the scheelite materialsCaMoO4,CaWO4,PbMoO4,andPbWO4. Physical Review B, 1998, 57, 12738-12750.	3.2	388
22	Orthogonal polynomial projectors for the projector augmented wave method of electronic structure calculations. Physical Review B, 1998, 57, 11827-11830.	3.2	18
23	Comparison of the projector augmented-wave, pseudopotential, and linearized augmented-plane-wave formalisms for density-functional calculations of solids. Physical Review B, 1997, 55, 2005-2017.	3.2	230
24	Density-functional calculation of the bulk and surface geometry of beryllium. Physical Review B, 1995, 51, 13653-13659.	3.2	33
25	Core-cancellation functions for evaluating exchange-correlation functionals in first-principles pseudopotential calculations. Physical Review B, 1994, 49, 2351-2361.	3.2	13
26	Density-functional calculation of the electronic structure and equilibrium geometry of iron pyrite (FeS2). Physical Review B, 1994, 50, 8214-8220.	3.2	40
27	Multilayer-relaxation geometry and electronic structure of a W(111) surface. Physical Review B, 1993, 48, 12136-12145.	3.2	22
28	Electronic structure of vacancy defects in MgO crystals. Physical Review B, 1990, 41, 3211-3225.	3.2	69
29	Spectral momentum density of graphite from (e,2e) spectroscopy: Comparison with first-principles calculation. Physical Review B, 1988, 37, 3914-3923.	3.2	41
30	Electronic structure ofKHgC4and related materials. Physical Review B, 1988, 38, 3722-3732.	3.2	7
31	Pseudopotential inversion scheme. Physical Review B, 1986, 33, 7139-7143.	3.2	8
32	Electronic structure ofRuS2. Physical Review B, 1985, 32, 3745-3752.	3.2	38
33	Interlayer states in graphite and in alkali-metal-graphite intercalation compounds. Physical Review B, 1984, 30, 2219-2222.	3.2	55
34	Local density pseudopotential calculations for molecules: O2 and Mo2O2S2(S2)2â^'2. Journal of Chemical Physics, 1984, 81, 3987-3995.	3.0	19
35	Electron momentum distribution in graphite and lithium-intercalated graphite. Physical Review B, 1984, 30, 1062-1064.	3.2	19
36	Energy-band structure and charge distribution for BaC6. International Journal of Quantum Chemistry, 1983, 23, 1223-1230.	2.0	22

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37	Lithium-intercalated graphite: Self-consistent electronic structure for stages one, two, and three. Physical Review B, 1983, 28, 1013-1025.	3.2	113
38	Local Spin-Density Description of Multiple Metal-Metal Bonding:Mo2andCr2. Physical Review Letters, 1983, 50, 1451-1454.	7.8	60
39	Density-functional study of interplanar binding in graphite. Physical Review B, 1983, 27, 2458-2469.	3.2	44
40	X-ray form factors and the electronic structure of graphite. Physical Review B, 1982, 26, 5382-5390.	3.2	202
41	Electronic Structure of Graphite Intercalation Compounds. Materials Research Society Symposia Proceedings, 1982, 20, 107.	0.1	0
42	Electronic Structure of Third-Stage Lithium Intercalated Graphite. Physical Review Letters, 1981, 47, 1318-1321.	7.8	16
43	Model Self-Consistent Bands for Graphite Intercalation Compounds. Springer Series in Solid-state Sciences, 1981, , 138-143.	0.3	0
44	Graphite intercalation compounds: A simple model of Fermi surface and transport properties. Physical Review B, 1980, 21, 3665-3674.	3.2	60
45	Surface electronic wave functions of a semi-infinite muffin-tin lattice. II. Application to Cu (001) and (110). Physical Review B, 1978, 18, 5365-5378.	3.2	8
46	Surface electronic wave functions of a semi-infinite muffin-tin lattice. I. The spherical-wave method. Physical Review B, 1978, 18, 5350-5364.	3.2	11
47	Theoretical study of lithium graphite. I. Band structure, density of states, and Fermi-surface properties. Physical Review B, 1978, 18, 5190-5205.	3.2	154
48	Magnetic Spin Susceptibility of AsF5-Intercalated Graphite: Determination of the Density of States at the Fermi Energy. Physical Review Letters, 1978, 41, 1417-1421.	7.8	73
49	Theoretical study of lithium graphite. II. Spatial distribution of valence electrons. Physical Review B, 1978, 18, 5206-5216.	3.2	55
50	Effects of spin-orbit interaction upon impurity scattering in dilute alloys. Physical Review B, 1976, 13, 2331-2341.	3.2	9
51	Electronic states of impurity atoms in noble-metal lattices. Physical Review B, 1976, 13, 3249-3260.	3.2	21
52	Theory of impurity scattering: Interstitial impurities. European Physical Journal B, 1975, 19, 161-170.	1.5	15
53	Theory of impurity scattering in dilute metal alloys based on the muffin-tin model. Physical Review B, 1975, 11, 3718-3738.	3.2	56
54	Nonrelativistic phase-shift analysis of impurity scattering in noble-metal hosts. Physical Review B, 1974, 10, 1213-1229.	3.2	98

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55	Mathieu function solutions to the radial SchrÃ¶dinger equation for the â^'f2/r4 interaction. Journal of Mathematical Physics, 1973, 14, 191-204.	1.1	43