

In-Ho Lee

List of Publications by Year in descending order

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73
papers

1,703
citations

257450

24
h-index

302126

39
g-index

74
all docs

74
docs citations

74
times ranked

1883
citing authors

#	ARTICLE	IF	CITATIONS
1	Applications of the generalized-gradient approximation to atoms, clusters, and solids. <i>Physical Review B</i> , 1997, 56, 7197-7205.	3.2	133
2	Two-dimensional limit of exchange-correlation energy functional approximations. <i>Physical Review B</i> , 2000, 61, 5202-5211.	3.2	129
3	Unbiased Global Optimization of Lennard-Jones Clusters for Using the Conformational Space Annealing Method. <i>Physical Review Letters</i> , 2003, 91, 080201.	7.8	115
4	Prediction of Green Phosphorus with Tunable Direct Band Gap and High Mobility. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4627-4632.	4.6	101
5	Shell filling of artificial atoms within density-functional theory. <i>Physical Review B</i> , 1998, 57, 9035-9042.	3.2	91
6	Computational search for direct band gap silicon crystals. <i>Physical Review B</i> , 2014, 90, .	3.2	63
7	Dynamics of Fullerene Coalescence. <i>Physical Review Letters</i> , 2003, 90, 065501.	7.8	59
8	Ab initio materials design using conformational space annealing and its application to searching for direct band gap silicon crystals. <i>Computer Physics Communications</i> , 2016, 203, 110-121.	7.5	55
9	Transition-pathway models of atomic diffusion on fcc metal surfaces. I. Flat surfaces. <i>Physical Review B</i> , 2007, 76, .	3.2	48
10	Transition-pathway models of atomic diffusion on fcc metal surfaces. II. Stepped surfaces. <i>Physical Review B</i> , 2007, 76, .	3.2	39
11	Superconducting Open-Framework Allotrope of Silicon at Ambient Pressure. <i>Physical Review Letters</i> , 2018, 120, 157001.	7.8	39
12	Electron-electron interactions in square quantum dots. <i>Physical Review B</i> , 2001, 63, .	3.2	37
13	Dipole-allowed direct band gap silicon superlattices. <i>Scientific Reports</i> , 2015, 5, 18086.	3.3	37
14	Protein structure modeling for CASP10 by multiple layers of global optimization. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 188-195.	2.6	36
15	Addition Spectra of Chaotic Quantum Dots: Interplay between Interactions and Geometry. <i>Physical Review Letters</i> , 1999, 83, 4144-4147.	7.8	34
16	Improvement of electron pump accuracy by a potential-shape-tunable quantum dot pump. <i>Physical Review B</i> , 2014, 90, .	3.2	34
17	One-way multigrid method in electronic-structure calculations. <i>Physical Review B</i> , 2000, 61, 4397-4400.	3.2	32
18	Uncertainty estimation of nanoparticle size distribution from a finite number of data obtained by microscopic analysis. <i>Metrologia</i> , 2009, 46, 480-488.	1.2	29

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19	Finding multiple reaction pathways via global optimization of action. Nature Communications, 2017, 8, 15443.	12.8	29
20	Atomic and electronic structure of amorphous Si from first-principles molecular-dynamics simulations. Physical Review B, 1994, 50, 18083-18089.	3.2	28
21	Template based protein structure modeling by global optimization in <sc>CASP</sc>11. Proteins: Structure, Function and Bioinformatics, 2016, 84, 221-232.	2.6	28
22	Molecular-dynamics study of melting on the shock Hugoniot of Al. Physical Review B, 1999, 59, 329-333.	3.2	27
23	Adatom-assisted structural transformations of fullerenes. Applied Physics Letters, 2006, 88, 011913.	3.3	26
24	Dynamic folding pathway models of α -helix and β -hairpin structures. Chemical Physics Letters, 2005, 412, 307-312.	2.6	25
25	Invariant-molecular-dynamics study of the diamond-to- β -Sn transition in Si under hydrostatic and uniaxial compressions. Physical Review B, 1997, 55, 5689-5693.	3.2	23
26	Lattice thermal conductivity of crystalline and amorphous silicon with and without isotopic effects from the ballistic to diffusive thermal transport regime. Journal of Applied Physics, 2014, 116, .	2.5	23
27	Kinetic energy control in action-derived molecular dynamics simulations. Physical Review B, 2003, 68, .	3.2	22
28	Dynamic folding pathway models of the villin headpiece subdomain (HP α 36) structure. Journal of Computational Chemistry, 2010, 31, 57-65.	3.3	22
29	Efficient modified Jacobi relaxation for minimizing the energy functional. Physical Review B, 1993, 47, 15996-15999.	3.2	21
30	A tight-binding molecular dynamics study of the equilibrium structures of small Si clusters. Journal of Physics Condensed Matter, 1994, 6, 741-750.	1.8	20
31	Design of Single-Layer Metasurface Filter by Conformational Space Annealing Algorithm for 5G mm-Wave Communications. IEEE Access, 2021, 9, 29764-29774.	4.2	20
32	Protein structure modeling and refinement by global optimization in CASP12. Proteins: Structure, Function and Bioinformatics, 2018, 86, 122-135.	2.6	19
33	Semimetallic carbon allotrope with a topological nodal line in mixed sp ² -sp ³ bonding networks. NPC Asia Materials, 2017, 9, e361-e361.	7.9	18
34	Reconstruction and alignment of vacancies in carbon nanotubes. Physical Review B, 2009, 79, .	3.2	16
35	Capacitive energies of quantum dots with hydrogenic impurity. Physical Review B, 1999, 60, 13720-13726.	3.2	15
36	Boron Triangular Kagome Lattice with Half-Metallic Ferromagnetism. Scientific Reports, 2017, 7, 7279.	3.3	14

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37	Dynamic pathway model for the formation of C60. <i>Journal of Chemical Physics</i> , 2004, 120, 4672-4676.	3.0	12
38	An introductory overview of action-derived molecular dynamics for multiple time-scale simulations. <i>Computer Methods in Applied Mechanics and Engineering</i> , 2004, 193, 1633-1644.	6.6	12
39	Folding Models of Mini-Protein FSD-1. <i>Journal of Physical Chemistry B</i> , 2012, 116, 6916-6922.	2.6	12
40	Direct band gap carbon superlattices with efficient optical transition. <i>Physical Review B</i> , 2016, 93, .	3.2	12
41	Electronic structure of ellipsoidally deformed quantum dots. <i>Journal of Physics Condensed Matter</i> , 2001, 13, 1987-1993.	1.8	11
42	Cooperative atomic motions and core rearrangement in dislocation cross slip. <i>Applied Physics Letters</i> , 2006, 88, 201908.	3.3	11
43	Electromechanical properties of alternating AlN and SiC nanoribbon sheets. <i>Computational Materials Science</i> , 2013, 78, 129-133.	3.0	11
44	Crystal structure prediction in a continuous representative space. <i>Computational Materials Science</i> , 2021, 194, 110436.	3.0	11
45	Symmetric stress tensor in the local-density-functional framework using a separable nonlocal pseudopotential. <i>Physical Review B</i> , 1995, 51, 14697-14700.	3.2	9
46	Dynamic Folding Pathway Models of the Trp-Cage Protein. <i>BioMed Research International</i> , 2013, 2013, 1-9.	1.9	9
47	Coalescence and T-junction formation of carbon nanotubes: Action-derived molecular dynamics simulations. <i>Physical Review B</i> , 2006, 74, .	3.2	8
48	Mobility of a 5 7 defect in carbon nanotubes. <i>Nanotechnology</i> , 2011, 22, 105707.	2.6	7
49	Design of dual-band single-layer metasurfaces for millimeter-wave 5G communication systems. <i>Applied Physics Letters</i> , 2021, 119, .	3.3	7
50	Object-oriented construction of a multigrid electronic-structure code with Fortran 90. <i>Computer Physics Communications</i> , 2000, 131, 10-25.	7.5	6
51	Strain-tunable half-metallicity in hybrid graphene-hBN monolayer superlattices. <i>Applied Surface Science</i> , 2016, 375, 179-185.	6.1	6
52	Quantum transport properties of single-crystalline Ag ₂ Se _{0.5} Te _{0.5} nanowires as a new topological material. <i>Nanoscale</i> , 2019, 11, 5171-5179.	5.6	6
53	First-principles study of the equilibrium structures of clusters. <i>Journal of Physics Condensed Matter</i> , 1998, 10, 5851-5860.	1.8	5
54	Searching Protein Folding Pathways by Optimization of Actions. <i>Journal of Computational and Theoretical Nanoscience</i> , 2009, 6, 2388-2392.	0.4	5

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55	Action-derived molecular dynamics simulations for the migration and coalescence of vacancies in graphene and carbon nanotubes. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 115303.	1.8	4
56	Three-dimensional buckled honeycomb boron lattice with vacancies as an intermediate phase on the transition pathway from I _± -B to I ³ -B. <i>NPG Asia Materials</i> , 2017, 9, e400-e400.	7.9	4
57	Self-Encapsulation of Silicene in Cubic Diamond Si: Topological Semimetal in Covalent Bonding Networks. <i>Journal of Physical Chemistry C</i> , 2019, 123, 1839-1845.	3.1	4
58	Dynamics of the Neuropeptide Met-Enkephalin by Using Action-Derived Molecular Dynamics. <i>Journal of the Korean Physical Society</i> , 2008, 53, 1764-1769.	0.7	4
59	Helix Formation of the Villin Headpiece Protein Subdomain. <i>Journal of the Korean Physical Society</i> , 2011, 59, 3321-3324.	0.7	4
60	Transition Pathway and Its Free-Energy Profile: A Protocol for Protein Folding Simulations. <i>International Journal of Molecular Sciences</i> , 2013, 14, 16058-16075.	4.1	3
61	Topological Invariant Prediction via Deep Learning. <i>Journal of the Korean Physical Society</i> , 2020, 76, 401-405.	0.7	3
62	Publisher's Note: Computational search for direct band gap silicon crystals [Phys. Rev. B90, 115209 (2014)]. <i>Physical Review B</i> , 2014, 90, .	3.2	2
63	CRFalign: A Sequence-Structure Alignment of Proteins Based on a Combination of HMM-HMM Comparison and Conditional Random Fields. <i>Molecules</i> , 2022, 27, 3711.	3.8	2
64	Hydrogen-beryllium complexes in crystalline silicon. <i>Physical Review B</i> , 1992, 46, 2041-2046.	3.2	1
65	Free-energy profile along an isomerization pathway: Conformational isomerization in alanine dipeptide. <i>Journal of the Korean Physical Society</i> , 2013, 62, 384-392.	0.7	1
66	Hydrophobic core of the villin headpiece protein. <i>Journal of the Korean Physical Society</i> , 2013, 63, 1234-1238.	0.7	1
67	Finding Dominant Reaction Pathways via Global Optimization of Action. <i>Biophysical Journal</i> , 2017, 112, 290a.	0.5	1
68	Action-Based Pathway Modeling for Atomic Surface Diffusion. <i>International Journal for Multiscale Computational Engineering</i> , 2007, 5, 273-286.	1.2	1
69	Optimum action method for the study of barrier-crossing events. <i>Journal of the Korean Physical Society</i> , 2009, 55, 2209-2217.	0.7	1
70	Potential-tunable quantum dot single-electron pump. , 2014, , .		0
71	A Folding Pathway Model of Mini-Protein BBA5. <i>BioMed Research International</i> , 2015, 2015, 1-9.	1.9	0
72	Finding Multiple Reaction Pathways via Global Optimization of Action. <i>Biophysical Journal</i> , 2019, 116, 303a.	0.5	0

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73	Ab initio prediction of nontrivial topological band and superconductivity in stable metallic Si allotropes at ambient pressure. <i>Physical Review Materials</i> , 2021, 5, .	2.4	0