In-Ho Lee

List of Publications by Year
in descending order

73 papers	1,703 citations	257101 24 h-index	301761 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. Physical Review B, 1997, 56, 7197-7205.	1.1	133
2	Two-dimensional limit of exchange-correlation energy functional approximations. Physical Review B, 2000, 61, 5202-5211.	1.1	129
3	Unbiased Global Optimization of Lennard-Jones Clusters forNâ‰201Using the Conformational Space Annealing Method. Physical Review Letters, 2003, 91, 080201.	2.9	115
4	Prediction of Green Phosphorus with Tunable Direct Band Gap and High Mobility. Journal of Physical Chemistry Letters, 2017, 8, 4627-4632.	2.1	101
5	Shell filling of artificial atoms within density-functional theory. Physical Review B, 1998, 57, 9035-9042.	1.1	91
6	Computational search for direct band gap silicon crystals. Physical Review B, 2014, 90, .	1.1	63
7	Dynamics of Fullerene Coalescence. Physical Review Letters, 2003, 90, 065501.	2.9	59
8	Ab initio materials design using conformational space annealing and its application to searching for direct band gap silicon crystals. Computer Physics Communications, 2016, 203, 110-121.	3.0	55
9	Transition-pathway models of atomic diffusion on fcc metal surfaces. I. Flat surfaces. Physical Review B, 2007, 76, .	1.1	48
10	Transition-pathway models of atomic diffusion on fcc metal surfaces. II. Stepped surfaces. Physical Review B, 2007, 76, .	1.1	39
11	Superconducting Open-Framework Allotrope of Silicon at Ambient Pressure. Physical Review Letters, 2018, 120, 157001.	2.9	39
12	Electron-electron interactions in square quantum dots. Physical Review B, 2001, 63, .	1.1	37
13	Dipole-allowed direct band gap silicon superlattices. Scientific Reports, 2015, 5, 18086.	1.6	37
14	Protein structure modeling for CASP10 by multiple layers of global optimization. Proteins: Structure, Function and Bioinformatics, 2014, 82, 188-195.	1.5	36
15	Addition Spectra of Chaotic Quantum Dots: Interplay between Interactions and Geometry. Physical Review Letters, 1999, 83, 4144-4147.	2.9	34
16	Improvement of electron pump accuracy by a potential-shape-tunable quantum dot pump. Physical Review B, 2014, 90, .	1.1	34
17	One-way multigrid method in electronic-structure calculations. Physical Review B, 2000, 61, 4397-4400.	1.1	32
18	Uncertainty estimation of nanoparticle size distribution from a finite number of data obtained by microscopic analysis. Metrologia, 2009, 46, 480-488.	0.6	29

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19	Finding multiple reaction pathways via global optimization of action. Nature Communications, 2017, 8, 15443.	5.8	29
20	Atomic and electronic structure of amorphous Si from first-principles molecular-dynamics simulations. Physical Review B, 1994, 50, 18083-18089.	1.1	28
21	Template based protein structure modeling by global optimization in <scp>CASP</scp>11. Proteins: Structure, Function and Bioinformatics, 2016, 84, 221-232.	1.5	28
22	Molecular-dynamics study of melting on the shock Hugoniot of Al. Physical Review B, 1999, 59, 329-333.	1.1	27
23	Adatom-assisted structural transformations of fullerenes. Applied Physics Letters, 2006, 88, 011913.	1.5	26
24	Dynamic folding pathway models of Î±-helix and Î²-hairpin structures. Chemical Physics Letters, 2005, 412, 307-312.	1.2	25
25	Invariant-molecular-dynamics study of the diamond-to-Î²-Sn transition in Si under hydrostatic and uniaxial compressions. Physical Review B, 1997, 55, 5689-5693.	1.1	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, .	1.1	23
27	Kinetic energy control in action-derived molecular dynamics simulations. Physical Review B, 2003, 68, .	1.1	22
28	Dynamic folding pathway models of the villin headpiece subdomain (HPâ€36) structure. Journal of Computational Chemistry, 2010, 31, 57-65.	1.5	22
29	Efficient modified Jacobi relaxation for minimizing the energy functional. Physical Review B, 1993, 47, 15996-15999.	1.1	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.	0.7	20
31	Design of Single-Layer Metasurface Filter by Conformational Space Annealing Algorithm for 5G mm-Wave Communications. IEEE Access, 2021, 9, 29764-29774.	2.6	20
32	Protein structure modeling and refinement by global optimization in CASP12. Proteins: Structure, Function and Bioinformatics, 2018, 86, 122-135.	1.5	19
33	Semimetallic carbon allotrope with a topological nodal line in mixed sp2-sp3 bonding networks. NPG Asia Materials, 2017, 9, e361-e361.	3.8	18
34	Reconstruction and alignment of vacancies in carbon nanotubes. Physical Review B, 2009, 79, .	1.1	16
35	Capacitive energies of quantum dots with hydrogenic impurity. Physical Review B, 1999, 60, 13720-13726.	1.1	15
36	Boron Triangular Kagome Lattice with Half-Metallic Ferromagnetism. Scientific Reports, 2017, 7, 7279.	1.6	14

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37	Dynamic pathway model for the formation of C60. Journal of Chemical Physics, 2004, 120, 4672-4676.	1.2	12
38	An introductory overview of action-derived molecular dynamics for multiple time-scale simulations. Computer Methods in Applied Mechanics and Engineering, 2004, 193, 1633-1644.	3.4	12
39	Folding Models of Mini-Protein FSD-1. Journal of Physical Chemistry B, 2012, 116, 6916-6922.	1.2	12
40	Direct band gap carbon superlattices with efficient optical transition. Physical Review B, 2016, 93, .	1.1	12
41	Electronic structure of ellipsoidally deformed quantum dots. Journal of Physics Condensed Matter, 2001, 13, 1987-1993.	0.7	11
42	Cooperative atomic motions and core rearrangement in dislocation cross slip. Applied Physics Letters, 2006, 88, 201908.	1.5	11
43	Electromechanical properties of alternating AlN and SiC nanoribbon sheets. Computational Materials Science, 2013, 78, 129-133.	1.4	11
44	Crystal structure prediction in a continuous representative space. Computational Materials Science, 2021, 194, 110436.	1.4	11
45	Symmetric stress tensor in the local-density-functional framework using a separable nonlocal pseudopotential. Physical Review B, 1995, 51, 14697-14700.	1.1	9
46	Dynamic Folding Pathway Models of the Trp-Cage Protein. BioMed Research International, 2013, 2013, 1-9.	0.9	9
47	Coalescence and T-junction formation of carbon nanotubes: Action-derived molecular dynamics simulations. Physical Review B, 2006, 74, .	1.1	8
48	Mobility of a 5|7 defect in carbon nanotubes. Nanotechnology, 2011, 22, 105707.	1.3	7
49	Design of dual-band single-layer metasurfaces for millimeter-wave 5G communication systems. Applied Physics Letters, 2021, 119, .	1.5	7
50	Object-oriented construction of a multigrid electronic-structure code with Fortran 90. Computer Physics Communications, 2000, 131, 10-25.	3.0	6
51	Strain-tunable half-metallicity in hybrid graphene-hBN monolayer superlattices. Applied Surface Science, 2016, 375, 179-185.	3.1	6
52	Quantum transport properties of single-crystalline Ag₂Se_{0.5}Te_{0.5} nanowires as a new topological material. Nanoscale, 2019, 11, 5171-5179.	2.8	6
53	First-principles study of the equilibrium structures of clusters. Journal of Physics Condensed Matter, 1998, 10, 5851-5860.	0.7	5
54	Searching Protein Folding Pathways by Optimization of Actions. Journal of Computational and Theoretical Nanoscience, 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. Journal of Physics Condensed Matter, 2014, 26, 115303.	0.7	4
56	Three-dimensional buckled honeycomb boron lattice with vacancies as an intermediate phase on the transition pathway from Î±-B to Î³-B. NPG Asia Materials, 2017, 9, e400-e400.	3.8	4
57	Self-Encapsulation of Silicene in Cubic Diamond Si: Topological Semimetal in Covalent Bonding Networks. Journal of Physical Chemistry C, 2019, 123, 1839-1845.	1.5	4
58	Dynamics of the Neuropeptide Met-Enkephalin by Using Action-Derived Molecular Dynamics. Journal of the Korean Physical Society, 2008, 53, 1764-1769.	0.3	4
59	Helix Formation of the Villin Headpiece Protein Subdomain. Journal of the Korean Physical Society, 2011, 59, 3321-3324.	0.3	4
60	Transition Pathway and Its Free-Energy Profile: A Protocol for Protein Folding Simulations. International Journal of Molecular Sciences, 2013, 14, 16058-16075.	1.8	3
61	Topological Invariant Prediction via Deep Learning. Journal of the Korean Physical Society, 2020, 76, 401-405.	0.3	3
62	Publisher's Note: Computational search for direct band gap silicon crystals [Phys. Rev. B90, 115209 (2014)]. Physical Review B, 2014, 90, .	1.1	2
63	CRFalign: A Sequence-Structure Alignment of Proteins Based on a Combination of HMM-HMM Comparison and Conditional Random Fields. Molecules, 2022, 27, 3711.	1.7	2
64	Hydrogen-beryllium complexes in crystalline silicon. Physical Review B, 1992, 46, 2041-2046.	1.1	1
65	Free-energy profile along an isomerization pathway: Conformational isomerization in alanine dipeptide. Journal of the Korean Physical Society, 2013, 62, 384-392.	0.3	1
66	Hydrophobic core of the villin headpiece protein. Journal of the Korean Physical Society, 2013, 63, 1234-1238.	0.3	1
67	Finding Dominant Reaction Pathways via Global Optimization of Action. Biophysical Journal, 2017, 112, 290a.	0.2	1
68	Action-Based Pathway Modeling for Atomic Surface Diffusion. International Journal for Multiscale Computational Engineering, 2007, 5, 273-286.	0.8	1
69	Optimum action method for the study of barrier-crossing events. Journal of the Korean Physical Society, 2009, 55, 2209-2217.	0.3	1
70	Potential-tunable quantum dot single-electron pump. , 2014, , .		0
71	A Folding Pathway Model of Mini-Protein BBA5. BioMed Research International, 2015, 2015, 1-9.	0.9	0
72	Finding Multiple Reaction Pathways via Global Optimization of Action. Biophysical Journal, 2019, 116, 303a.	0.2	0

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73	Ab initio prediction of nontrivial topological band and superconductivity in stable metallic Si allotropes at ambient pressure. Physical Review Materials, 2021, 5, .	0.9	0