

Kwiseon Kim

List of Publications by Year in descending order

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31
papers

2,350
citations

471061

17
h-index

525886

27
g-index

31
all docs

31
docs citations

31
times ranked

2808
citing authors

#	ARTICLE	IF	CITATIONS
1	Elastic constants and related properties of tetrahedrally bonded BN, AlN, GaN, and InN. <i>Physical Review B</i> , 1996, 53, 16310-16326.	1.1	670
2	First-principles study of native defects in anataseTiO2. <i>Physical Review B</i> , 2006, 73, .	1.1	346
3	Electronic structure of GaN with strain and phonon distortions. <i>Physical Review B</i> , 1994, 50, 1502-1505.	1.1	198
4	Theoretical Studies on Conjugated Phenyl-Cored Thiophene Dendrimers for Photovoltaic Applications. <i>Journal of the American Chemical Society</i> , 2007, 129, 14257-14270.	6.6	190
5	Hydroxide Degradation Pathways for Substituted Trimethylammonium Cations: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 9419-9426.	1.5	176
6	Finding Gas Diffusion Pathways in Proteins: Application to O2 and H2 Transport in Cpl [FeFe]-Hydrogenase and the Role of Packing Defects. <i>Structure</i> , 2005, 13, 1321-1329.	1.6	170
7	Molecular Dynamics Simulations of Proton Transport in 3M and Nafion Perfluorosulfonic Acid Membranes. <i>Journal of Physical Chemistry C</i> , 2013, 117, 8079-8091.	1.5	91
8	Divacancy-nitrogen-assisted transition metal dispersion and hydrogen adsorption in defective graphene: A first-principles study. <i>Physical Review B</i> , 2010, 81, .	1.1	90
9	Density Functional Theory Calculation of Bonding and Charge Parameters for Molecular Dynamics Studies on [FeFe] Hydrogenases. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1137-1145.	2.3	76
10	Shape Dependence of Band-Edge Exciton Fine Structure in CdSe Nanocrystals. <i>Nano Letters</i> , 2007, 7, 3274-3280.	4.5	47
11	Charge Transport Simulations in Conjugated Dendrimers. <i>Journal of Physical Chemistry A</i> , 2010, 114, 4388-4393.	1.1	43
12	Atomic Resolution Modeling of the Ferredoxin:[FeFe] Hydrogenase Complex from <i>Chlamydomonas reinhardtii</i> . <i>Biophysical Journal</i> , 2007, 93, 3034-3045.	0.2	39
13	Brownian Dynamics and Molecular Dynamics Study of the Association between Hydrogenase and Ferredoxin from <i>Chlamydomonas reinhardtii</i> . <i>Biophysical Journal</i> , 2008, 95, 3753-3766.	0.2	38
14	Exciton Migration in Conjugated Dendrimers: A Joint Experimental and Theoretical Study. <i>ChemPhysChem</i> , 2009, 10, 3285-3294.	1.0	31
15	Hydrogenase/Ferredoxin Charge-Transfer Complexes: Effect of Hydrogenase Mutations on the Complex Association. <i>Journal of Physical Chemistry A</i> , 2009, 113, 4060-4067.	1.1	29
16	Surface passivation optimization using DIRECT. <i>Journal of Computational Physics</i> , 2007, 224, 824-835.	1.9	21
17	Electronic and Optical Properties of the Group-III Nitrides, their Heterostructures and Alloys. <i>Materials Research Society Symposia Proceedings</i> , 1995, 395, 455.	0.1	20
18	Thermal conductance at atomically clean and disordered silicon/aluminum interfaces: A molecular dynamics simulation study. <i>Journal of Applied Physics</i> , 2012, 112, .	1.1	16

#	ARTICLE	IF	CITATIONS
19	Negative band gap bowing in epitaxial InAs/GaAs alloys and predicted band offsets of the strained binaries and alloys on various substrates. Applied Physics Letters, 2002, 80, 3105-3107.	1.5	14
20	Elastic Constants and Related Properties of the Group III-Nitrides. Materials Research Society Symposia Proceedings, 1995, 395, 399.	0.1	11
21	Band Structure and Cation Ordering in LiGaO ₂ . Materials Research Society Symposia Proceedings, 1996, 449, 905.	0.1	7
22	Characterization Of Bulk, Polycrystalline Indium Nitride Grown At Sub-Atmospheric Pressures. Materials Research Society Symposia Proceedings, 1997, 482, 593.	0.1	7
23	Predicting the electronic properties of 3D, million-atom semiconductor nanostructure architectures. Journal of Physics: Conference Series, 2006, 46, 292-298.	0.3	7
24	Direct enumeration studies of band-gap properties of Al _x Ga _{1-x} In _y P alloys. Journal of Applied Physics, 2009, 105, 123531.	1.1	5
25	Theoretical Study of Group-III-Nitride Alloys. Materials Research Society Symposia Proceedings, 1996, 449, 929.	0.1	3
26	NanoPSE: Nanoscience Problem Solving Environment for atomistic electronic structure of semiconductor nanostructures. Journal of Physics: Conference Series, 2005, 16, 277-282.	0.3	3
27	Data Mining-Aided Crystal Engineering for the Design of Transparent Conducting Oxides. Materials Research Society Symposia Proceedings, 2011, 1315, 1.	0.1	1
28	Molecular Dynamics Modeling of Thermal Conductance at Atomically Clean and Disordered Silicon/Aluminum Interfaces. , 2011, , .		1
29	Material Design via Genetic Algorithms for Semiconductor Alloys and Superlattices. AIP Conference Proceedings, 2005, , .	0.3	0
30	Numerical Formulation of the Effective Medium Approximation: Illustrative Examples and Application to Organic Semiconductors. Materials Research Society Symposia Proceedings, 2009, 1177, 25.	0.1	0
31	Molecular Dynamics Modeling of Heat Transport in Metals and Semiconductors. , 2010, , .		0