Kwiseon Kim

List of Publications by Year
in descending order

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31	2,350	471061	525886
papers	citations	17 h-index	27 g-index

31	31	31	2808
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular Dynamics Simulations of Proton Transport in 3M and Nafion Perfluorosulfonic Acid Membranes. Journal of Physical Chemistry C, 2013, 117, 8079-8091.	1.5	91
2	Thermal conductance at atomically clean and disordered silicon/aluminum interfaces: A molecular dynamics simulation study. Journal of Applied Physics, 2012, 112, .	1.1	16
3	Hydroxide Degradation Pathways for Substituted Trimethylammonium Cations: A DFT Study. Journal of Physical Chemistry C, 2012, 116, 9419-9426.	1.5	176
4	Data Mining-Aided Crystal Engineering for the Design of Transparent Conducting Oxides. Materials Research Society Symposia Proceedings, 2011, 1315, 1.	0.1	1
5	Molecular Dynamics Modeling of Thermal Conductance at Atomically Clean and Disordered Silicon/Aluminum Interfaces. , 2011, , .		1
6	Molecular Dynamics Modeling of Heat Transport in Metals and Semiconductors. , 2010, , .		0
7	Charge Transport Simulations in Conjugated Dendrimers. Journal of Physical Chemistry A, 2010, 114, 4388-4393.	1.1	43
8	Divacancy-nitrogen-assisted transition metal dispersion and hydrogen adsorption in defective graphene: A first-principles study. Physical Review B, 2010, 81, .	1.1	90
9	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
10	Exciton Migration in Conjugated Dendrimers: A Joint Experimental and Theoretical Study. ChemPhysChem, 2009, 10, 3285-3294.	1.0	31
11	Density Functional Theory Calculation of Bonding and Charge Parameters for Molecular Dynamics Studies on [FeFe] Hydrogenases. Journal of Chemical Theory and Computation, 2009, 5, 1137-1145.	2.3	76
12	Direct enumeration studies of band-gap properties of AlxGayIn1â^'xâ^'yP alloys. Journal of Applied Physics, 2009, 105, 123531.	1.1	5
13	Hydrogenase/Ferredoxin Charge-Transfer Complexes: Effect of Hydrogenase Mutations on the Complex Association. Journal of Physical Chemistry A, 2009, 113, 4060-4067.	1.1	29
14	Brownian Dynamics and Molecular Dynamics Study of the Association between Hydrogenase and Ferredoxin from Chlamydomonas reinhardtii. Biophysical Journal, 2008, 95, 3753-3766.	0.2	38
15	Theoretical Studies on Conjugated Phenyl-Cored Thiophene Dendrimers for Photovoltaic Applications. Journal of the American Chemical Society, 2007, 129, 14257-14270.	6.6	190
16	Atomic Resolution Modeling of the Ferredoxin:[FeFe] Hydrogenase Complex from Chlamydomonas reinhardtii. Biophysical Journal, 2007, 93, 3034-3045.	0.2	39
17	Surface passivation optimization using DIRECT. Journal of Computational Physics, 2007, 224, 824-835.	1.9	21
18	Shape Dependence of Band-Edge Exciton Fine Structure in CdSe Nanocrystals. Nano Letters, 2007, 7, 3274-3280.	4.5	47

#	Article	IF	Citations
19	First-principles study of native defects in anataseTiO2. Physical Review B, 2006, 73, .	1.1	346
20	Predicting the electronic properties of 3D, million-atom semiconductor nanostructure architectures. Journal of Physics: Conference Series, 2006, 46, 292-298.	0.3	7
21	NanoPSE: Nanoscience Problem Solving Environment for atomistic electronic structure of semiconductor nanostructures. Journal of Physics: Conference Series, 2005, 16, 277-282.	0.3	3
22	Finding Gas Diffusion Pathways in Proteins: Application to O2 and H2 Transport in CpI [FeFe]-Hydrogenase and the Role of Packing Defects. Structure, 2005, 13, 1321-1329.	1.6	170
23	Material Design via Genetic Algorithms for Semiconductor Alloys and Superlattices. AIP Conference Proceedings, 2005, , .	0.3	0
24	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
25	Characterization Of Bulk, Polycrystalline Indium Nitride Grown At Sub-Atmospheric Pressures. Materials Research Society Symposia Proceedings, 1997, 482, 593.	0.1	7
26	Elastic constants and related properties of tetrahedrally bonded BN, AlN, GaN, and InN. Physical Review B, 1996, 53, 16310-16326.	1.1	670
27	Band Structure and Cation Ordering in LiGaO₂. Materials Research Society Symposia Proceedings, 1996, 449, 905.	0.1	7
28	Theoretical Study of Group-III-Nitride Alloys. Materials Research Society Symposia Proceedings, 1996, 449, 929.	0.1	3
29	Electronic and Optical Properties of the Group-III Nitrides, their Heterostructures and Alloys. Materials Research Society Symposia Proceedings, 1995, 395, 455.	0.1	20
30	Elastic Constants and Related Properties of the Group III-Nitrides. Materials Research Society Symposia Proceedings, 1995, 395, 399.	0.1	11
31	Electronic structure of GaN with strain and phonon distortions. Physical Review B, 1994, 50, 1502-1505.	1.1	198