Sung Sakong

List of Publications by Year
in descending order

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49 papers	2,154 citations	218677 26 h-index	223800 46 g-index
52 all docs	52 docs citations	52 times ranked	2612 citing authors

#	Article	IF	Citations
1	Structure of PtRu/Ru(0Â0Â0Â1) and AgPd/Pd(1Â1Â1) surface alloys: A kinetic Monte Carlo study. Chemical Physics, 2022, 555, 111428.	1.9	4
2	Ab Initio Simulations of Water/Metal Interfaces. Chemical Reviews, 2022, 122, 10746-10776.	47.7	72
3	The structure of the electric double layer: Atomistic versus continuum approaches. Current Opinion in Electrochemistry, 2022, 33, 100953.	4.8	7
4	In Search of the Active Sites for the Selective Catalytic Reduction on Tungsten-Doped Vanadia Monolayer Catalysts Supported by TiO₂. ACS Catalysis, 2021, 11, 7411-7421.	11.2	14
5	The Dynamic Nature of CO Adlayers on Pt(111) Electrodes. Angewandte Chemie - International Edition, 2020, 59, 6182-6186.	13.8	20
6	Influence of Local Inhomogeneities and the Electrochemical Environment on the Oxygen Reduction Reaction on Pt-Based Electrodes: A DFT Study. Journal of Physical Chemistry C, 2020, 124, 27604-27613.	3.1	10
7	Diffusion on a Crowded Surface: kMC Simulations. Journal of Physical Chemistry C, 2020, 124, 15216-15224.	3.1	9
8	The Dynamic Nature of CO Adlayers on Pt(111) Electrodes. Angewandte Chemie, 2020, 132, 6241-6245.	2.0	5
9	Water structures on a Pt(111) electrode from ab initio molecular dynamic simulations for a variety of electrochemical conditions. Physical Chemistry Chemical Physics, 2020, 22, 10431-10437.	2.8	65
10	Improved DFT Adsorption Energies with Semiempirical Dispersion Corrections. Journal of Chemical Theory and Computation, 2019, 15, 3250-3259.	5.3	43
11	Density fluctuations as door-opener for diffusion on crowded surfaces. Science, 2019, 363, 715-718.	12.6	32
12	Modelling the electric double layer at electrode/electrolyte interfaces. Current Opinion in Electrochemistry, 2019, 14, 1-6.	4.8	93
13	Reaction energetics of hydrogen on Si(100) surface: A periodic many-electron theory study. Journal of Chemical Physics, 2018, 149, 244105.	3.0	11
14	The electric double layer at metal-water interfaces revisited based on a charge polarization scheme. Journal of Chemical Physics, 2018, 149, 084705.	3.0	128
15	Influence of Step and Island Edges on Local Adsorption Properties: Hydrogen Adsorption on Pt Monolayer Island Modified Ru(0001) Electrodes. Electrocatalysis, 2017, 8, 530-539.	3.0	9
16	Methanol Oxidation on Pt(111) from First-Principles in Heterogeneous and Electrocatalysis. Electrocatalysis, 2017, 8, 577-586.	3.0	26
17	The structure of water at a Pt(111) electrode and the potential of zero charge studied from first principles. Journal of Chemical Physics, 2016, 144, 194701.	3.0	127
18	The Importance of the Electrochemical Environment in the Electro-Oxidation of Methanol on Pt(111). ACS Catalysis, 2016, 6, 5575-5586.	11.2	117

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19	Unoccupied electronic structure and momentum-dependent scattering dynamics in Pb/Si(557) nanowire arrays. Physical Review B, 2015, 92, .	3.2	4
20	Density functional theory study of the electrochemical interface between a Pt electrode and an aqueous electrolyte using an implicit solvent method. Journal of Chemical Physics, 2015, 142, 234107.	3.0	103
21	Some challenges in the first-principles modeling of structures and processes in electrochemical energy storage and transfer. Journal of Power Sources, 2015, 275, 531-538.	7.8	49
22	Electronic and Structural Differences between Wurtzite and Zinc Blende InAs Nanowire Surfaces: Experiment and Theory. ACS Nano, 2014, 8, 12346-12355.	14.6	78
23	Interplay of hydrogen treatment and nitrogen doping in ZnO nanoparticles: a first-principles study. Nanotechnology, 2014, 25, 145204.	2.6	7
24	Water Structures at Metal Electrodes Studied by Ab Initio Molecular Dynamics Simulations. Journal of the Electrochemical Society, 2014, 161, E3015-E3020.	2.9	81
25	Interface defects and impurities at the growth zone of Auâ€catalyzed GaAs nanowire from first principles. Physica Status Solidi - Rapid Research Letters, 2013, 7, 882-885.	2.4	1
26	Comparison of density functionals for nitrogen impurities in ZnO. Journal of Chemical Physics, 2013, 138, 234702.	3.0	13
27	Atomistic modeling of the Au dropletâ€“GaAs interface for size-selective nanowire growth. Physical Review B, 2013, 88, .	3.2	21
28	Mode conversion and long-lived vibrational modes in lead monolayers on silicon (111) after femtosecond laser excitation: A molecular dynamics simulation. Physical Review B, 2013, 88, .	3.2	15
29	As vacancies, Ga antisites, and Au impurities in zinc blende and wurtzite GaAs nanowire segments from first principles. Physical Review B, 2013, 87, .	3.2	27
30	Anisotropic ferromagnetism in carbon-doped zinc oxide from first-principles studies. Physical Review B, 2012, 86, .	3.2	31
31	Role of sidewall diffusion in GaAs nanowire growth: A first-principles study. Physical Review B, 2012, 86, .	3.2	25
32	Lowering Energy Barriers in Surface Reactions through Concerted Reaction Mechanisms. ChemPhysChem, 2012, 13, 3467-3471.	2.1	19
33	Catalytic Role of Gold Nanoparticle in GaAs Nanowire Growth: A Density Functional Theory Study. Nano Letters, 2012, 12, 943-948.	9.1	30
34	Density functional study of carbon doping in ZnO. Semiconductor Science and Technology, 2011, 26, 014038.	2.0	24
35	Calculation of the diameter-dependent polytypism in GaAs nanowires from an atomic motif expansion of the formation energy. Physical Review B, 2011, 84, .	3.2	53
36	Isotopic effect on the vibrational lifetime of the carbon-deuterium stretch excitation on graphene. Journal of Chemical Physics, 2011, 135, 114506.	3.0	5

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37	Hydrogen vibrational modes on graphene and relaxation of the Câ€“H stretch excitation from first-principles calculations. Journal of Chemical Physics, 2010, 133, 054505.	3.0	40
38	Magnetism in C- or N-doped MgO and ZnO: A Density-Functional Study of Impurity Pairs. Physical Review Letters, 2010, 105, 267203.	7.8	111
39	Isotope effects in the vibrational lifetime of hydrogen on germanium(100): Theory and experiment. Journal of Chemical Physics, 2009, 131, 124502.	3.0	13
40	Density-functional theory study of vibrational relaxation of CO stretching excitation on Si(100). Journal of Chemical Physics, 2008, 129, 174702.	3.0	27
41	Energetics driving the short-range order in CuxPd1â€“x/Ru(0001) monolayer surface alloys. Physical Chemistry Chemical Physics, 2007, 9, 5127.	2.8	22
42	Total Oxidation of Methanol on Cu(110):Â A Density Functional Theory Study. Journal of Physical Chemistry A, 2007, 111, 8814-8822.	2.5	74
43	CO adsorption on Cuâ€“Pd alloy surfaces: ligand versus ensemble effects. Physical Chemistry Chemical Physics, 2007, 9, 2216-2225.	2.8	79
44	Local density of states effects at the metal-molecule interfaces in a molecular device. Nature Materials, 2006, 5, 394-399.	27.5	98
45	Kinetic Monte Carlo simulations of the partial oxidation of methanol on oxygen-covered Cu(110). Surface Science, 2006, 600, 3258-3265.	1.9	32
46	Partial oxidation of methanol on Cu(110): Energetics and kinetics. Computational and Theoretical Chemistry, 2006, 771, 117-122.	1.5	22
47	Quantum dynamics of the dissociation of H2 on Rh(111). European Physical Journal B, 2005, 45, 425-432.	1.5	9
48	Density functional theory study of the partial oxidation of methanol on copper surfaces. Journal of Catalysis, 2005, 231, 420-429.	6.2	102
49	Dissociative adsorption of hydrogen on strained Cu surfaces. Surface Science, 2003, 525, 107-118.	1.9	147