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	Dissociative adsorption of hydrogen on strained Cu surfaces. Surface Science, 2003, 525, 107-118.	1.9	147
2	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
3	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
4	The Importance of the Electrochemical Environment in the Electro-Oxidation of Methanol on Pt(111). ACS Catalysis, 2016, 6, 5575-5586.	11.2	117
5	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
6	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
7	Density functional theory study of the partial oxidation of methanol on copper surfaces. Journal of Catalysis, 2005, 231, 420-429.	6.2	102
8	Local density of states effects at the metal-molecule interfaces in a molecular device. Nature Materials, 2006, 5, 394-399.	27.5	98
9	Modelling the electric double layer at electrode/electrolyte interfaces. Current Opinion in Electrochemistry, 2019, 14, 1-6.	4.8	93
10	Water Structures at Metal Electrodes Studied by Ab Initio Molecular Dynamics Simulations. Journal of the Electrochemical Society, 2014, 161, E3015-E3020.	2.9	81
11	CO adsorption on Cuâ€“Pd alloy surfaces: ligand versus ensemble effects. Physical Chemistry Chemical Physics, 2007, 9, 2216-2225.	2.8	79
12	Electronic and Structural Differences between Wurtzite and Zinc Blende InAs Nanowire Surfaces: Experiment and Theory. ACS Nano, 2014, 8, 12346-12355.	14.6	78
13	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
14	Ab Initio Simulations of Water/Metal Interfaces. Chemical Reviews, 2022, 122, 10746-10776.	47.7	72
15	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
16	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
17	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
18	Improved DFT Adsorption Energies with Semiempirical Dispersion Corrections. Journal of Chemical Theory and Computation, 2019, 15, 3250-3259.	5.3	43

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19	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
20	Kinetic Monte Carlo simulations of the partial oxidation of methanol on oxygen-covered Cu(110). Surface Science, 2006, 600, 3258-3265.	1.9	32
21	Density fluctuations as door-opener for diffusion on crowded surfaces. Science, 2019, 363, 715-718.	12.6	32
22	Anisotropic ferromagnetism in carbon-doped zinc oxide from first-principles studies. Physical Review B, 2012, 86, .	3.2	31
23	Catalytic Role of Gold Nanoparticle in GaAs Nanowire Growth: A Density Functional Theory Study. Nano Letters, 2012, 12, 943-948.	9.1	30
24	Density-functional theory study of vibrational relaxation of CO stretching excitation on Si(100). Journal of Chemical Physics, 2008, 129, 174702.	3.0	27
25	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
26	Methanol Oxidation on Pt(111) from First-Principles in Heterogeneous and Electrocatalysis. Electrocatalysis, 2017, 8, 577-586.	3.0	26
27	Role of sidewall diffusion in GaAs nanowire growth: A first-principles study. Physical Review B, 2012, 86, .	3.2	25
28	Density functional study of carbon doping in ZnO. Semiconductor Science and Technology, 2011, 26, 014038.	2.0	24
29	Partial oxidation of methanol on Cu(110): Energetics and kinetics. Computational and Theoretical Chemistry, 2006, 771, 117-122.	1.5	22
30	Energetics driving the short-range order in CuxPd1â€“x/Ru(0001) monolayer surface alloys. Physical Chemistry Chemical Physics, 2007, 9, 5127.	2.8	22
31	Atomistic modeling of the Au dropletâ€“GaAs interface for size-selective nanowire growth. Physical Review B, 2013, 88, .	3.2	21
32	The Dynamic Nature of CO Adlayers on Pt(111) Electrodes. Angewandte Chemie - International Edition, 2020, 59, 6182-6186.	13.8	20
33	Lowering Energy Barriers in Surface Reactions through Concerted Reaction Mechanisms. ChemPhysChem, 2012, 13, 3467-3471.	2.1	19
34	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
35	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
36	Isotope effects in the vibrational lifetime of hydrogen on germanium(100): Theory and experiment. Journal of Chemical Physics, 2009, 131, 124502.	3.0	13

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37	Comparison of density functionals for nitrogen impurities in ZnO. Journal of Chemical Physics, 2013, 138, 234702.	3.0	13
38	Reaction energetics of hydrogen on Si(100) surface: A periodic many-electron theory study. Journal of Chemical Physics, 2018, 149, 244105.	3.0	11
39	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
40	Quantum dynamics of the dissociation of H2 on Rh(111). European Physical Journal B, 2005, 45, 425-432.	1.5	9
41	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
42	Diffusion on a Crowded Surface: kMC Simulations. Journal of Physical Chemistry C, 2020, 124, 15216-15224.	3.1	9
43	Interplay of hydrogen treatment and nitrogen doping in ZnO nanoparticles: a first-principles study. Nanotechnology, 2014, 25, 145204.	2.6	7
44	The structure of the electric double layer: Atomistic versus continuum approaches. Current Opinion in Electrochemistry, 2022, 33, 100953.	4.8	7
45	Isotopic effect on the vibrational lifetime of the carbon-deuterium stretch excitation on graphene. Journal of Chemical Physics, 2011, 135, 114506.	3.0	5
46	The Dynamic Nature of CO Adlayers on Pt(111) Electrodes. Angewandte Chemie, 2020, 132, 6241-6245.	2.0	5
47	Unoccupied electronic structure and momentum-dependent scattering dynamics in Pb/Si(557) nanowire arrays. Physical Review B, 2015, 92, .	3.2	4
48	Structure of PtRu/Ru(0Â0Â0Â1) and AgPd/Pd(1Â1Â1) surface alloys: A kinetic Monte Carlo study. Chemical Physics, 2022, 555, 111428.	1.9	4
49	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