

Johannes Frenzel

List of Publications by Year in descending order

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Version: 2024-02-01

27
papers

1,211
citations

471509

17
h-index

580821

25
g-index

29
all docs

29
docs citations

29
times ranked

2053
citing authors

#	ARTICLE	IF	CITATIONS
1	Atomic-Scale Explanation of O ₂ Activation at the Au–TiO ₂ Interface. <i>Journal of the American Chemical Society</i> , 2018, 140, 18082-18092.	13.7	69
2	Bicanonical <i>ab Initio</i> Molecular Dynamics for Open Systems. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3455-3469.	5.3	10
3	Heterogeneous Catalysis on Metal/Oxide Systems from Accelerated <i>Ab Initio</i> Simulations. <i>Advanced Science Letters</i> , 2017, 23, 5834-5836.	0.2	0
4	Reaction Network of Methanol Synthesis over Cu/ZnO Nanocatalysts. <i>ACS Catalysis</i> , 2015, 5, 4201-4218.	11.2	87
5	Efficient Calculation of Electronic Absorption Spectra by Means of Intensity-Selected Time-Dependent Density Functional Tight Binding. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 157-167.	5.3	42
6	Cu/ZnO nanocatalysts in response to environmental conditions: surface morphology, electronic structure, redox state and CO ₂ activation. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26119-26136.	2.8	17
7	Methanol synthesis on ZnO($\overline{111}$). IV. Reaction mechanisms and electronic structure. <i>Journal of Chemical Physics</i> , 2014, 141, 124710.	3.0	18
8	Methanol synthesis on ZnO($\overline{111}$). II. Structure, energetics, and vibrational signature of reaction intermediates. <i>Journal of Chemical Physics</i> , 2013, 139, 044705.	3.0	16
9	Tuning the Reactivity of a Cu/ZnO Nanocatalyst via Gas Phase Pressure. <i>Physical Review Letters</i> , 2013, 110, 086108.		31
10	Methanol synthesis on ZnO from molecular dynamics. <i>Physica Status Solidi (B): Basic Research</i> , 2013, 250, 1174-1190.	1.5	16
11	Electronic structure calculations of large cadmium chalcogenide nanoparticles. <i>Physica Status Solidi (B): Basic Research</i> , 2012, 249, 384-391.	1.5	2
12	Structural properties of metal-organic frameworks within the density functional based tight-binding method. <i>Physica Status Solidi (B): Basic Research</i> , 2012, 249, 335-342.	1.5	42
13	Do Cement Nanotubes exist?. <i>Advanced Materials</i> , 2012, 24, 3239-3245.	21.0	51
14	Methanol synthesis on ZnO($\overline{001}$). III. Free energy landscapes, reaction pathways, and mechanistic insights. <i>Journal of Chemical Physics</i> , 2011, 134, 064710.	3.0	33
15	Optical Excitations in CdSe/CdS Core–Shell Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2011, 115, 10338-10344.	3.1	7
16	On the reticular construction concept of covalent organic frameworks. <i>Beilstein Journal of Nanotechnology</i> , 2010, 1, 60-70.	2.8	139
17	Adsorption of nucleotides on the rutile (110) surface. <i>International Journal of Materials Research</i> , 2010, 101, 758-764.	0.3	22
18	Surface Effects in the Pressure-Induced Structural Transformation of a ZnO Nanorod. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2009, 635, 1773-1776.	1.2	9

#	ARTICLE	IF	CITATIONS
19	Adsorption of Phosphonic Acid at the TiO ₂ Anatase (101) and Rutile (110) Surfaces. Journal of Physical Chemistry C, 2009, 113, 5730-5740.	3.1	155
20	Adsorption of phosphonic and ethylphosphonic acid on aluminum oxide surfaces. Surface Science, 2008, 602, 1347-1359.	1.9	97
21	Optical Excitations in Cadmium Sulfide Nanoparticles. Journal of Physical Chemistry C, 2007, 111, 10761-10770.	3.1	57
22	Imogolite Nanotubes: Stability, Electronic, and Mechanical Properties. ACS Nano, 2007, 1, 362-368.	14.6	172
23	The Effects of Organisation, Embedding and Surfactants on the Properties of Cadmium Chalcogenide (CdS, CdSe and CdS/CdSe) Semiconductor Nanoparticles. European Journal of Inorganic Chemistry, 2005, 2005, 3585-3596.	2.0	33
24	Structural and Electronic Properties of Bulk Gibbsite and Gibbsite Surfaces. ChemInform, 2005, 36, no.	0.0	0
25	The Effects of Organization, Embedding and Surfactants on the Properties of Cadmium Chalcogenide (CdS, CdSe and CdS/CdSe) Semiconductor Nanoparticles. ChemInform, 2005, 36, no.	0.0	0
26	Structural and Electronic Properties of Bulk Gibbsite and Gibbsite Surfaces. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2005, 631, 1267-1271.	1.2	63
27	Electronic structure of Ga ₈₄ cluster compounds. Physical Review B, 2004, 70, .	3.2	15