Ari P Seitsonen

List of Publications by Year
in descending order

186 papers	36,836 citations	22153 59 h-index	3650 180 g-index
190 all docs	190 docs citations	190 times ranked	32703 citing authors

#	Article	IF	Citations
1	Gold speciation in hydrothermal fluids revealed by in situ high energy resolution X-ray absorption spectroscopy. American Mineralogist, 2022, 107, 369-376.	1.9	8
2	Field emission microscope for a single fullerene molecule. Scientific Reports, 2022, 12, 2714.	3.3	4
3	First steps of blue phosphorene growth on Au(1 1 1). Materials Today: Proceedings, 2021, 39, 1153-1156.	1.8	4
4	Fluorescent silica MCM-41 nanoparticles based on flavonoids: Direct post-doping encapsulation and spectral characterization. Dyes and Pigments, 2021, 185, 108870.	3.7	3
5	Interaction of cyclosporin A molecules with alkali and transition metal atoms on Cu(111). Chemical Communications, 2021, 57, 2923-2926.	4.1	2
6	Tunable Interface of Ruthenium Porphyrins and Silver. Journal of Physical Chemistry C, 2021, 125, 3215-3224.	3.1	14
7	Electron spectroscopies of 3-hydroxyflavone and 7-hydroxyflavone in MCM-41 silica nanoparticles and in acetonitrile solutions. Experimental data and DFT/TD-DFT calculations. Data in Brief, 2021, 34, 106630.	1.0	1
8	Assembly and Manipulation of a Prototypical N-Heterocyclic Carbene with a Metalloporphyrin Pedestal on a Solid Surface. Journal of the American Chemical Society, 2021, 143, 4433-4439.	13.7	18
9	Atomistic investigation of surface characteristics and electronic features at high-purity FeSi(110) presenting interfacial metallicity. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	5
10	Conformational Control of Chemical Reactivity for Surfaceâ€Confined Ruâ€Porphyrins. Angewandte Chemie, 2021, 133, 16697-16703.	2.0	2
11	Conformational Control of Chemical Reactivity for Surfaceâ€Confined Ruâ€Porphyrins. Angewandte Chemie - International Edition, 2021, 60, 16561-16567.	13.8	12
12	Grapheneâ€“Ionic Liquid Interfacial Potential Drop from Density Functional Theory-Based Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2020, 124, 19548-19555.	3.1	24
13	Characterization of molecular-atomic transformation in fluid hydrogen under pressure via long-wavelength asymptote of charge density fluctuations. Journal of Molecular Liquids, 2020, 312, 113274.	4.9	6
14	Charge State Control of F 16 CoPc on h â€BN/Cu(111). Advanced Materials Interfaces, 2020, 7, 2000080.	3.7	7
15	Understanding the Superior Stability of Singleâ€Molecule Magnets on an Oxide Film. Advanced Science, 2019, 6, 1901736.	11.2	36
16	Synthesizing Highly Regular Single-Layer Alkynylâ€“Silver Networks at the Micrometer Scale via Gas-Mediated Surface Reaction. Journal of the American Chemical Society, 2019, 141, 5087-5091.	13.7	30
17	Bottom-Up Fabrication of a Metal-Supported Oxoâ€“Metal Porphyrin. Journal of Physical Chemistry C, 2019, 123, 31011-31025.	3.1	12
18	Solvent effects on the vibrational spectrum of 3-hydroxyflavone. Journal of Molecular Liquids, 2019, 275, 723-728.	4.9	10

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19	Giant dichroism and angular deviation in x-ray absorption spectra of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Dy</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mathvariant="normal">C</mml:mi><mml:mn>80</mml:mn></mml:msub></mml:mrow></mml:math> single-molecule magnets on <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>h</mml:mi><mml:mtext>â˜’</mml:mtext><mml:mi>BN</mml:mi></mml:mrow></mml:math>. Physical Review Materials, 2019, 3, .	2.4	12
20	Benchmarking van der Waals-treated DFT: The case of hexagonal boron nitride and graphene on Ir(111). Physical Review Materials, 2019, 3, .	2.4	12
21	Metalation of Porphyrins by Lanthanide Atoms at Interfaces: Direct Observation and Stimulation of Cerium Coordination to 2H-TPP/Ag(111). Journal of Physical Chemistry C, 2018, 122, 5083-5092.	3.1	17
22	Lanthanide-Directed Assembly of Interfacial Coordination Architecturesâ€“From Complex Networks to Functional Nanosystems. Accounts of Chemical Research, 2018, 51, 365-375.	15.6	54
23	Complex supramolecular interfacial tessellation through convergent multi-step reaction of a dissymmetric simple organic precursor. Nature Chemistry, 2018, 10, 296-304.	13.6	68
24	Epitaxial Synthesis of Blue Phosphorene. Small, 2018, 14, e1804066.	10.0	114
25	Elemental Identification by Combining Atomic Force Microscopy and Kelvin Probe Force Microscopy. ACS Nano, 2018, 12, 5274-5283.	14.6	37
26	Electrostatic Interaction across a Single-Layer Carbon Shell. Journal of Physical Chemistry Letters, 2018, 9, 3586-3590.	4.6	6
27	An electron acceptor molecule in a nanomesh: F4TCNQ on h-BN/Rh(111). Surface Science, 2018, 678, 183-188.	1.9	8
28	Epitaxy-Induced Assembly and Enantiomeric Switching of an On-Surface Formed Dinuclear Organocobalt Complex. ACS Nano, 2017, 11, 1347-1359.	14.6	8
29	Sensitivity of photoelectron diffraction to conformational changes of adsorbed molecules: Tetra-tert-butyl-azobenzene/Au(111). Structural Dynamics, 2017, 4, 015101.	2.3	3
30	N-Heterocyclic carbenes on close-packed coinage metal surfaces: bis-carbene metal adatom bonding scheme of monolayer films on Au, Ag and Cu. Chemical Science, 2017, 8, 8301-8308.	7.4	87
31	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	1.8	4,303
32	Corrugation in the Weakly Interacting Hexagonal-BN/Cu(111) System: Structure Determination by Combining Noncontact Atomic Force Microscopy and X-ray Standing Waves. ACS Nano, 2017, 11, 9151-9161.	14.6	56
33	Melting temperature of water: DFT-based molecular dynamics simulations with D3 dispersion correction. Physical Review B, 2016, 94, .	3.2	15
34	Isomerism of Trimeric Aluminum Complexes in Aqueous Environments: Exploration via DFT-Based Metadynamics Simulation. Journal of Physical Chemistry B, 2016, 120, 11800-11809.	2.6	2
35	Electronic structure of reconstructed Au(111) studied with density functional theory. Surface Science, 2016, 643, 150-155.	1.9	7
36	Dispersion effects in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> An ab initio study. Physical Review B, 2015, 92, .	3.2	27

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37	Proton disorder in cubic ice: Effect on the electronic and optical properties. Journal of Chemical Physics, 2015, 143, 084507.	3.0	7
38	Carbon dioxide in silicate melts at upper mantle conditions: Insights from atomistic simulations. Chemical Geology, 2015, 418, 77-88.	3.3	29
39	Combined experiment and theory approach in surface chemistry: Stairway to heaven?. Surface Science, 2015, 640, 165-180.	1.9	22
40	Functionalization of CeO₂(1â€‰1â€‰1) by Deposition of Small Ni Clusters: Effects on CO₂ Adsorption and O Vacancy Formation. ChemCatChem, 2015, 7, 625-634.	3.7	31
41	Many-body transitions in a single molecule visualized by scanning tunnelling microscopy. Nature Physics, 2015, 11, 229-234.	16.7	63
42	Chiral modification of platinum: ab initio study of the effect of hydrogen coadsorption on stability and geometry of adsorbed cinchona alkaloids. Physical Chemistry Chemical Physics, 2015, 17, 27615-27629.	2.8	16
43	Pressure-induced emergence of unusually high-frequency transverse excitations in a liquid alkali metal: Evidence of two types of collective excitations contributing to the transverse dynamics at high pressures. Journal of Chemical Physics, 2015, 143, 104502.	3.0	32
44	Sulfur radical species form gold deposits on Earth. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 13484-13489.	7.1	107
45	Chemical Reactions on Metal-supported Hexagonal Boron Nitride Investigated with Density Functional Theory. Chimia, 2014, 68, 596.	0.6	9
46	Epitaxial hexagonal boron nitride on Ir(111): A work function template. Physical Review B, 2014, 89, .	3.2	85
47	Self-Assembly and Chemical Modifications of Bisphenol A on Cu(111): Interplay Between Ordering and Thermally Activated Stepwise Deprotonation. ACS Nano, 2014, 8, 207-215.	14.6	31
48	Control of Molecular Organization and Energy Level Alignment by an Electronically Nanopatterned Boron Nitride Template. ACS Nano, 2014, 8, 430-442.	14.6	75
49	Five-Vertex Lanthanide Coordination on Surfaces: A Route to Sophisticated Nanoarchitectures and Tessellations. Journal of Physical Chemistry C, 2014, 118, 12908-12915.	3.1	34
50	Structure, equation of state and transport properties of molten calcium carbonate (CaCO3) by atomistic simulations. Geochimica Et Cosmochimica Acta, 2014, 141, 547-566.	3.9	56
51	Formation, migration, and clustering of point defects in CuInSe₂from first principles. Journal of Physics Condensed Matter, 2014, 26, 345501.	1.8	31
52	Charge-density correlations in pressurized liquid lithium calculated usingab initiomolecular dynamics. Physical Review B, 2014, 90, .	3.2	9
53	Dehalogenation and Coupling of a Polycyclic Hydrocarbon on an Atomically Thin Insulator. ACS Nano, 2014, 8, 6571-6579.	14.6	44
54	Hexagonal boron nitride on transition metal surfaces. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	93

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55	Dynamical Crossover at the Liquid-Liquid Transformation of a Compressed Molten Alkali Metal. Physical Review Letters, 2013, 111, 077801.	7.8	28
56	Effect of sodium incorporation into CuInSe2 from first principles. Journal of Applied Physics, 2013, 114, .	2.5	67
57	Coverage Effect of the CO₂ Adsorption Mechanisms on CeO₂(111) by First Principles Analysis. Journal of Physical Chemistry C, 2013, 117, 1701-1711.	3.1	103
58	Silver in geological fluids from in situ X-ray absorption spectroscopy and first-principles molecular dynamics. Geochimica Et Cosmochimica Acta, 2013, 106, 501-523.	3.9	44
59	Extracting chemical information from plane wave calculations by a 3D â€˜fuzzy atomsâ€™ analysis. Chemical Physics Letters, 2013, 563, 97-101.	2.6	9
60	Structural and electronic properties of a large-scale MoirÃ© pattern of hexagonal boron nitride on Cu(111) studied with density functional theory. Nanoscale, 2013, 5, 5589.	5.6	34
61	Photoelectron diffraction in the x-ray and ultraviolet regime: Sn-phthalocyanine on Ag(111). Physical Review B, 2013, 87, .	3.2	17
62	Five-vertex Archimedean surface tessellation by lanthanide-directed molecular self-assembly. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 6678-6681.	7.1	123
63	Combined ARPES and STM study of Pb/Au(111) MoirÃ© structure: One overlayer, two symmetries. Physical Review B, 2013, 87, .	3.2	13
64	Mass transport in CuInSe2 from first principles. Journal of Applied Physics, 2013, 113, .	2.5	22
65	Topic 14+16: High-Performance and Scientific Applications and Extreme-Scale Computing. Lecture Notes in Computer Science, 2013, , 737-738.	1.3	0
66	Electronic Structure of an Organic/Metal Interface: Pentacene/Cu(110). Journal of Physical Chemistry C, 2012, 116, 23465-23471.	3.1	49
67	Hierarchically Organized Bimolecular Ladder Network Exhibiting Guided One-Dimensional Diffusion. ACS Nano, 2012, 6, 549-556.	14.6	12
68	Chemical Transformations Drive Complex Self-Assembly of Uracil on Close-Packed Coinage Metal Surfaces. ACS Nano, 2012, 6, 2477-2486.	14.6	55
69	Redirecting focus in CuInSe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>research towards selenium-related defects. Physical Review B, 2012, 86, .	3.2	26
70	Adsorption of chlorine on Ru(0001)â€”A combined density functional theory and quantitative low energy electron diffraction study. Surface Science, 2012, 606, 297-304.	1.9	13
71	Hidden polymorphs drive vitrification in B2O3. Nature Materials, 2012, 11, 925-929.	27.5	60
72	Nature of the attractive interaction between proton acceptors and organic ring systems. Physical Chemistry Chemical Physics, 2012, 14, 15995.	2.8	53

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73	Adsorption of silicon on Au(110): An ordered two dimensional surface alloy. Applied Physics Letters, 2012, 101, .	3.3	34
74	Structure and Dynamics of Liquid Water from ab Initio Molecular Dynamicsâ€"Comparison of BLYP, PBE, and revPBE Density Functionals with and without van der Waals Corrections. Journal of Chemical Theory and Computation, 2012, 8, 3902-3910.	5.3	247
75	Boron Nitride on Cu(111): An Electronically Corrugated Monolayer. Nano Letters, 2012, 12, 5821-5828.	9.1	187
76	From molten salts to room temperature ionic liquids: Simulation studies on chloroaluminate systems. Faraday Discussions, 2012, 154, 171-188.	3.2	59
77	Selective Supramolecular Fullereneâ€"Porphyrin Interactions and Switching in Surface-Confined C60â€"Ce(TPP)2 Dyads. Nano Letters, 2012, 12, 4077-4083.	9.1	46
78	Effect of Dispersion on the Structure and Dynamics of the Ionic Liquid 1â€Ethylâ€3â€methylimidazolium Thiocyanate. ChemPhysChem, 2012, 13, 1845-1853.	2.1	81
79	A review on silicene â€" New candidate for electronics. Surface Science Reports, 2012, 67, 1-18.	7.2	707
80	â€œFirstâ€Principlesâ€kinetic monte carlo simulations revisited: CO oxidation over RuO₂(110). Journal of Computational Chemistry, 2012, 33, 757-766.	3.3	43
81	Structure and Dynamics of Liquid Water from ab Initio Molecular Dynamicsâ€"Comparison of BLYP, PBE, and revPBE Density Functionals with and without van der Waals Corrections. Journal of Chemical Theory and Computation, 2012, 8, 3902-3910.	5.3	116
82	Growth and characterization of fullerene nanocrystals on NaCl/Au(111). Physical Review B, 2011, 84, .	3.2	44
83	Van der Waals effects in ab initio water at ambient and supercritical conditions. Journal of Chemical Physics, 2011, 135, 154503.	3.0	138
84	Vacancies in CuInSe₂: new insights from hybrid-functional calculations. Journal of Physics Condensed Matter, 2011, 23, 422202.	1.8	25
85	Structure and stability of graphene nanoribbons in oxygen, carbon dioxide, water, and ammonia. Physical Review B, 2010, 82, .	3.2	85
86	Electronic and optical properties of group IV twoâ€dimensional materials. Physica Status Solidi (A) Applications and Materials Science, 2010, 207, 291-299.	1.8	21
87	Atomically precise bottom-up fabrication of graphene nanoribbons. Nature, 2010, 466, 470-473.	27.8	3,144
88	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Si</mml:mtext></mml:mrow><mml:mtext>C</mml:mtext></mml pairs in SiC identified as paramagnetic defects with strongly anisotropic orbital quenching. Physical Review B, 2010, 81, .	3.2	15
89	Strong3p-T1uhybridization inAr@C60. Physical Review A, 2010, 82, .	2.5	14
90	Site-specific electronic and geometric interface structure of Co-tetraphenyl-porphyrin layers on Ag(111). Physical Review B, 2010, 81, .	3.2	124

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91	First-principles theory of orbital magnetization. Physical Review B, 2010, 81, .	3.2	77
92	Hydrogen-Promoted Chlorination of RuO₂(110). Journal of Physical Chemistry C, 2010, 114, 10901-10909.	3.1	25
93	Oxidation of HCl over TiO₂-Supported RuO₂: A Density Functional Theory Study. Journal of Physical Chemistry C, 2010, 114, 22624-22629.	3.1	42
94	Clarâ€™s Theory, Ï€-Electron Distribution, and Geometry of Graphene Nanoribbons. Journal of the American Chemical Society, 2010, 132, 3440-3451.	13.7	219
95	Dynamic response of chlorine atoms on a RuO2(110) model catalyst surface. Physical Chemistry Chemical Physics, 2010, 12, 15358.	2.8	28
96	Deacon Process over RuO2 and TiO2-Supported RuO2. , 2010, , 517-528.		0
97	First-principles calculations of x-ray absorption in a scheme based on ultrasoft pseudopotentials: From<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-quartz to high-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>T</mml:mi><mml:mi>c</mml:mi></mml:msub></mml:mrow></mml:math>com	3.2	150
98	Si_CC_{Si}Antisite Pairs as Dominant Irradiation Induced Defects in p-Type 4H-SiC. Materials Science Forum, 2009, 615-617, 357-360.	0.3	5
99	Kondo-effect of substitutional cobalt impurities at copper surfaces. New Journal of Physics, 2009, 11, 113015.	2.9	20
100	Intimate interplay of theory and experiments in model catalysis. Surface Science, 2009, 603, 1717-1723.	1.9	30
101	The thermodynamic stability and simulated STM images of graphene nanoribbons. Physica Status Solidi (B): Basic Research, 2009, 246, 2586-2591.	1.5	9
102	Supramolecular control of the magnetic anisotropy inÂtwo-dimensional high-spin Fe arrays at a metalÂinterface. Nature Materials, 2009, 8, 189-193.	27.5	262
103	Reaction mechanism of ammonia oxidation over RuO2(110): A combined theory/experiment approach. Surface Science, 2009, 603, L113-L116.	1.9	21
104	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics Condensed Matter, 2009, 21, 395502.	1.8	18,183
105	Intrinsic charge transfer gap in NiO from<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mtext>Ni</mml:mtext><mml:mtext>â€‰</mml:mtext><mml:mi>K</mml:mi></mml:math>-edge x-ray absorption spectroscopy. Physical Review B, 2009, 79, .	3.2	72
106	Importance of van der Waals Interactions in Liquid Water. Journal of Physical Chemistry B, 2009, 113, 1127-1131.	2.6	175
107	Unexpected Hydrogen Bond Dynamics in Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2009, 113, 15129-15132.	2.6	112
108	Oxidative Dehydrogenation of Simple Molecules over RuO2(110): Density Functional Theory Calculations. , 2009, , 187-199.		0

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109	Ga self-interstitials in GaN investigated byab-initio calculations of the electronicg -tensor. Physica Status Solidi (B): Basic Research, 2008, 245, 924-926.	1.5	13
110	Stable Deacon Process for HCl Oxidation over RuO₂. Angewandte Chemie - International Edition, 2008, 47, 2131-2134.	13.8	123
111	Structure, Stability, Edge States, and Aromaticity of Graphene Ribbons. Physical Review Letters, 2008, 101, 096402.	7.8	582
112	Interaction of Cerium Atoms with Surface-Anchored Porphyrin Molecules. Journal of Physical Chemistry C, 2008, 112, 3453-3455.	3.1	81
113	X-ray linear dichroism in cubic compounds: The case of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mrow><mml:mtext>Cr</mml:mtext></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mr xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>MgAl</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:m Physical Review B, 2008, 78, .	3.2	50
114	Reaction Mechanism of the Oxidation of HCl over RuO₂(110). Journal of Physical Chemistry C, 2008, 112, 9966-9969.	3.1	68
115	Boroxol Rings in Liquid and Vitreous<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>from First Principles. Physical Review Letters, 2008, 101, 065504.	7.8	131
116	Heterogeneous oxidation catalysis on ruthenium: bridging the pressure and materials gaps and beyond. Journal of Physics Condensed Matter, 2008, 20, 184017.	1.8	57
117	Teraflops Sustained Performance With Real World Applications. International Journal of High Performance Computing Applications, 2008, 22, 131-148.	3.7	1
118	Electronic structure at the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:math>/metal interface: An angle-resolved photoemission and first-principles study. Physical Review B, 2008, 77, .	3.2	59
119	Green Chemistry from Supercomputers: Car-Parrinello Simulations of Emim-Chloroaluminates Ionic Liquids. , 2008, , 213-227.		1
120	Green Chemistry from Supercomputers: Carâ€“Parrinello Simulations of Emim-Chloroaluminates Ionic Liquids. , 2008, , 157-171.		0
121	Complex Interaction of Hydrogen with the RuO2(110) Surface. Journal of Physical Chemistry C, 2007, 111, 5363-5373.	3.1	88
122	Ionic Liquids from Carâ^'Parrinello Simulations. 2. Structural Diffusion Leading to Large Anions in Chloraluminate Ionic Liquids. Inorganic Chemistry, 2007, 46, 2751-2754.	4.0	53
123	Buckybowls on Metal Surfaces: Symmetry Mismatch and Enantiomorphism of Corannulene on Cu(110). Angewandte Chemie - International Edition, 2007, 46, 8258-8261.	13.8	81
124	Comment on â€œCO oxidation on ruthenium: The nature of the active catalytic surfaceâ€•by D.W. Goodman, C.H.F. Peden, M.S. Chen. Surface Science, 2007, 601, 5659-5662.	1.9	44
125	Green Chemistry from Supercomputers: Car-Parrinello Simulations for Ionic Liquids. , 2007, , 135-144.		0
126	Electronic structure of an orderedPbâ^•Ag(111)surface alloy: Theory and experiment. Physical Review B, 2006, 73, .	3.2	92

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127	Molecular Dynamics Simulation of Liquid Water:Â Hybrid Density Functionalsâ€. Journal of Physical Chemistry B, 2006, 110, 3685-3691.	2.6	242
128	Comment on â€œInteraction of Hydrogen with RuO2(110) Surfaces:Â Activity Differences between Various Oxygen Speciesâ€• Journal of Physical Chemistry B, 2006, 110, 22947-22947.	2.6	18
129	Unusual Process of Water Formation on RuO2(110) by Hydrogen Exposure at Room Temperature. Journal of Physical Chemistry B, 2006, 110, 14007-14010.	2.6	35
130	Density Functional Theory Analysis of Carboxylate-Bridged Diiron Units in Two-Dimensional Metalâˆ’Organic Grids. Journal of the American Chemical Society, 2006, 128, 5634-5635.	13.7	93
131	Ionic Liquids from Carâˆ’Parrinello Simulations, Part I:Â Liquid AlCl3. Journal of Physical Chemistry B, 2006, 110, 11475-11480.	2.6	31
132	Asymmetry Induction by Cooperative Intermolecular Hydrogen Bonds in Surface-Anchored Layers of Achiral Molecules. ChemPhysChem, 2006, 7, 2197-2204.	2.1	46
133	Ultrathin Rh films on Ru(0001): Oxidation in confinement. Journal of Chemical Physics, 2006, 124, 034706.	3.0	1
134	Large dispersion of incoherent spectral features in highly orderedC60chains. Physical Review B, 2006, 74, .	3.2	16
135	Understanding the Structural Deactivation of Ruthenium Catalysts on an Atomic Scale under both Oxidizing and Reducing Conditions. Angewandte Chemie, 2005, 117, 939-942.	2.0	17
136	Understanding the Structural Deactivation of Ruthenium Catalysts on an Atomic Scale under both Oxidizing and Reducing Conditions. Angewandte Chemie - International Edition, 2005, 44, 917-920.	13.8	91
137	LEED and DFT investigation on the (2Ã—2)-S overlayer on Co(0001). Surface Science, 2005, 599, 113-121.	1.9	22
138	Irregular stacking sequence in the initial growth of ultrathin Rh films on Ru(0001). Physical Review B, 2005, 72, .	3.2	5
139	Doping-induced reorientation ofC60molecules on Ag(111). Physical Review B, 2005, 72, .	3.2	23
140	Rocking-motion-induced charging ofC60onhâˆ’BNâˆ•Ni(111). Physical Review B, 2005, 71, .	3.2	33
141	Hydrogen Transfer Reaction on the Surface of an Oxide Catalyst. Journal of the American Chemical Society, 2005, 127, 3236-3237.	13.7	69
142	Visualization of Atomic Processes on Ruthenium Dioxide using Scanning Tunneling Microscopy. ChemPhysChem, 2004, 5, 167-174.	2.1	67
143	The adsorption structure on Co{0001}: a combined Tensor LEED and DFT study. Surface Science, 2004, 572, 1-10.	1.9	13
144	STM Study of Terephthalic Acid Self-Assembly on Au(111):Â Hydrogen-Bonded Sheets on an Inhomogeneous Substrateâ€. Journal of Physical Chemistry B, 2004, 108, 14585-14590.	2.6	173

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147	Catalytic activity of RuO2(1 1 0) in the oxidation of CO. Catalysis Today, 2003, 85, 167-175.	4.4	54
148	Ruthenium Dioxide, a Versatile Oxidation Catalyst: First Principles Analysis. , 2003, , 177-187.		5
149	(3Ã—3)R30Â°â˜'(K+CO)coadsorption structure on Pt(111):â€ƒExperiment and theory. Physical Review B, 2002, 66, .	3.2	5
150	SURFACE CHEMISTRY: Oxidation of Metal Surfaces. Science, 2002, 297, 2003-2005.	12.6	169
151	On the origin of the Ru-3d5/2 satellite feature from RuO2(). Surface Science, 2002, 504, L196-L200.	1.9	72
152	Complex redox chemistry on the RuO2() surface: experiment and theory. Surface Science, 2002, 505, 137-152.	1.9	56
153	Experimental and simulated STM images of stoichiometric and partially reduced RuO2() surfaces including adsorbates. Surface Science, 2002, 515, 143-156.	1.9	67
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