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	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
2	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	1.8	4,303
3	Atomically precise bottom-up fabrication of graphene nanoribbons. Nature, 2010, 466, 470-473.	27.8	3,144
4	Atomic-Scale Structure and Catalytic Reactivity of the RuO2(110) Surface. Science, 2000, 287, 1474-1476.	12.6	829
5	A review on silicene â€" New candidate for electronics. Surface Science Reports, 2012, 67, 1-18.	7.2	707
6	Structure, Stability, Edge States, and Aromaticity of Graphene Ribbons. Physical Review Letters, 2008, 101, 096402.	7.8	582
7	Supramolecular control of the magnetic anisotropy inÂtwo-dimensional high-spin Fe arrays at a metalÂinterface. Nature Materials, 2009, 8, 189-193.	27.5	262
8	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
9	Molecular Dynamics Simulation of Liquid Water:Â Hybrid Density Functionalsâ€. Journal of Physical Chemistry B, 2006, 110, 3685-3691.	2.6	242
10	Clarâ€™s Theory, Ï€-Electron Distribution, and Geometry of Graphene Nanoribbons. Journal of the American Chemical Society, 2010, 132, 3440-3451.	13.7	219
11	Characterization of Various Oxygen Species on an Oxide Surface:â€‰ RuO2(110). Journal of Physical Chemistry B, 2001, 105, 3752-3758.	2.6	209
12	Boron Nitride on Cu(111): An Electronically Corrugated Monolayer. Nano Letters, 2012, 12, 5821-5828.	9.1	187
13	Real-space electronic-structure calculations: Combination of the finite-difference and conjugate-gradient methods. Physical Review B, 1995, 51, 14057-14061.	3.2	185
14	Importance of van der Waals Interactions in Liquid Water. Journal of Physical Chemistry B, 2009, 113, 1127-1131.	2.6	175
15	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
16	Strain dependence of surface diffusion: Ag on Ag(111) and Pt(111). Physical Review B, 1997, 55, 6750-6753.	3.2	171
17	SURFACE CHEMISTRY: Oxidation of Metal Surfaces. Science, 2002, 297, 2003-2005.	12.6	169
18	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>compou Physical Review B, 2009, 80, .	3.2	150

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19	Van der Waals effects in ab initio water at ambient and supercritical conditions. Journal of Chemical Physics, 2011, 135, 154503.	3.0	138
20	Electron-positron Car-Parrinello methods: Self-consistent treatment of charge densities and ionic relaxations. Physical Review B, 1995, 52, 10947-10961.	3.2	134
21	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
22	Site-specific electronic and geometric interface structure of Co-tetraphenyl-porphyrin layers on Ag(111). Physical Review B, 2010, 81, .	3.2	124
23	Stable Deacon Process for HCl Oxidation over RuO₂. Angewandte Chemie - International Edition, 2008, 47, 2131-2134.	13.8	123
24	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
25	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
26	Epitaxial Synthesis of Blue Phosphorene. Small, 2018, 14, e1804066.	10.0	114
27	Unexpected Hydrogen Bond Dynamics in Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2009, 113, 15129-15132.	2.6	112
28	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
29	New Bonding Configuration on Si(111) and Ge(111) Surfaces Induced by the Adsorption of Alkali Metals. Physical Review Letters, 1998, 80, 3980-3983.	7.8	104
30	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
31	Density Functional Theory Analysis of Carboxylate-Bridged Diiron Units in Two-Dimensional Metalâ^'Organic Grids. Journal of the American Chemical Society, 2006, 128, 5634-5635.	13.7	93
32	Hexagonal boron nitride on transition metal surfaces. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	93
33	Electronic structure of an orderedPbâ^•Ag(111)surface alloy: Theory and experiment. Physical Review B, 2006, 73, .	3.2	92
34	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
35	Complex Interaction of Hydrogen with the RuO2(110) Surface. Journal of Physical Chemistry C, 2007, 111, 5363-5373.	3.1	88
36	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

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37	Structure and stability of graphene nanoribbons in oxygen, carbon dioxide, water, and ammonia. Physical Review B, 2010, 82, .	3.2	85
38	Epitaxial hexagonal boron nitride on Ir(111): A work function template. Physical Review B, 2014, 89, .	3.2	85
39	Buckybowls on Metal Surfaces: Symmetry Mismatch and Enantiomorphism of Corannulene on Cu(110). Angewandte Chemie - International Edition, 2007, 46, 8258-8261.	13.8	81
40	Interaction of Cerium Atoms with Surface-Anchored Porphyrin Molecules. Journal of Physical Chemistry C, 2008, 112, 3453-3455.	3.1	81
41	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
42	The adsorption of atomic nitrogen on Ru(0001): geometry and energetics. Chemical Physics Letters, 1997, 264, 680-686.	2.6	77
43	First-principles theory of orbital magnetization. Physical Review B, 2010, 81, .	3.2	77
44	Large atomic displacements associated with the nitrogen antisite in GaN. Physical Review B, 1996, 54, 1474-1477.	3.2	76
45	Bonding Mechanism and Atomic Geometry of an Ordered Hydroxyl Overlayer on Pt(111). Journal of the American Chemical Society, 2001, 123, 7347-7351.	13.7	76
46	Control of Molecular Organization and Energy Level Alignment by an Electronically Nanopatterned Boron Nitride Template. ACS Nano, 2014, 8, 430-442.	14.6	75
47	The atomic geometry of oxygen-rich Ru(0001) surfaces: coexistence of (1Ã—1)O and RuO2(110) domains. Surface Science, 2000, 465, 1-8.	1.9	74
48	Epitaxial Growth of RuO2(100) on Ru(101Ì„0):â€‰ Surface Structure and Other Properties. Journal of Physical Chemistry B, 2001, 105, 2205-2211.	2.6	72
49	On the origin of the Ru-3d5/2 satellite feature from RuO2(). Surface Science, 2002, 504, L196-L200.	1.9	72
50	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
51	Hydrogen Transfer Reaction on the Surface of an Oxide Catalyst. Journal of the American Chemical Society, 2005, 127, 3236-3237.	13.7	69
52	Oxygen adsorption on the Ru(101Â¯0) surface: Anomalous coverage dependence. Physical Review B, 1998, 57, 15487-15495.	3.2	68
53	Reaction Mechanism of the Oxidation of HCl over RuO₂(110). Journal of Physical Chemistry C, 2008, 112, 9966-9969.	3.1	68
54	Complex supramolecular interfacial tessellation through convergent multi-step reaction of a dissymmetric simple organic precursor. Nature Chemistry, 2018, 10, 296-304.	13.6	68

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55	Experimental and simulated STM images of stoichiometric and partially reduced RuO2() surfaces including adsorbates. Surface Science, 2002, 515, 143-156.	1.9	67
56	Visualization of Atomic Processes on Ruthenium Dioxide using Scanning Tunneling Microscopy. ChemPhysChem, 2004, 5, 167-174.	2.1	67
57	Effect of sodium incorporation into CuInSe2 from first principles. Journal of Applied Physics, 2013, 114, .	2.5	67
58	Indium and phosphorus vacancies and antisites in InP. Physical Review B, 1994, 49, 5253-5262.	3.2	63
59	Many-body transitions in a single molecule visualized by scanning tunnelling microscopy. Nature Physics, 2015, 11, 229-234.	16.7	63
60	Spectroscopic characterization of catalytically active surface sites of a metallic oxide. Chemical Physics Letters, 2001, 342, 467-472.	2.6	61
61	Hidden polymorphs drive vitrification in B2O3. Nature Materials, 2012, 11, 925-929.	27.5	60
62	Direct Imaging of Catalytically Important Processes in the Oxidation of CO over RuO2(110). Journal of the American Chemical Society, 2001, 123, 11807-11808.	13.7	59
63	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
64	From molten salts to room temperature ionic liquids: Simulation studies on chloroaluminate systems. Faraday Discussions, 2012, 154, 171-188.	3.2	59
65	Comprehensive characterization of the (2Ã—2)-O and the CO-induced overlayers on Pd(111). Surface Science, 2000, 468, 176-186.	1.9	57
66	Heterogeneous oxidation catalysis on ruthenium: bridging the pressure and materials gaps and beyond. Journal of Physics Condensed Matter, 2008, 20, 184017.	1.8	57
67	Complex redox chemistry on the RuO2() surface: experiment and theory. Surface Science, 2002, 505, 137-152.	1.9	56
68	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
69	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
70	Chemical Transformations Drive Complex Self-Assembly of Uracil on Close-Packed Coinage Metal Surfaces. ACS Nano, 2012, 6, 2477-2486.	14.6	55
71	Catalytic activity of RuO2(1 1 0) in the oxidation of CO. Catalysis Today, 2003, 85, 167-175.	4.4	54
72	Lanthanide-Directed Assembly of Interfacial Coordination Architecturesâ€“From Complex Networks to Functional Nanosystems. Accounts of Chemical Research, 2018, 51, 365-375.	15.6	54

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73	Ionic Liquids from Carâˆ'Parrinello Simulations. 2. Structural Diffusion Leading to Large Anions in Chloraluminate Ionic Liquids. Inorganic Chemistry, 2007, 46, 2751-2754.	4.0	53
74	Nature of the attractive interaction between proton acceptors and organic ring systems. Physical Chemistry Chemical Physics, 2012, 14, 15995.	2.8	53
75	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> 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:mrow> Physical Review B, 2008, 78, .	3.2	50
76	Electronic Structure of an Organic/Metal Interface: Pentacene/Cu(110). Journal of Physical Chemistry C, 2012, 116, 23465-23471.	3.1	49
77	Positron annihilation in II-VI compound semiconductors: theory. Journal of Physics Condensed Matter, 1994, 6, 8809-8827.	1.8	46
78	Catalytic Activity of the RuO2(100) Surface in the Oxidation of COâ€. Journal of Physical Chemistry B, 2004, 108, 14392-14397.	2.6	46
79	Asymmetry Induction by Cooperative Intermolecular Hydrogen Bonds in Surface-Anchored Layers of Achiral Molecules. ChemPhysChem, 2006, 7, 2197-2204.	2.1	46
80	Selective Supramolecular Fullereneâ€“Porphyrin Interactions and Switching in Surface-Confined C60â€“Ce(TPP)2 Dyads. Nano Letters, 2012, 12, 4077-4083.	9.1	46
81	CO adsorption on the reducedRuO2(110)surface: Energetics and structure. Physical Review B, 2001, 65, .	3.2	44
82	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
83	Growth and characterization of fullerene nanocrystals on NaCl/Au(111). Physical Review B, 2011, 84, .	3.2	44
84	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
85	Dehalogenation and Coupling of a Polycyclic Hydrocarbon on an Atomically Thin Insulator. ACS Nano, 2014, 8, 6571-6579.	14.6	44
86	â€œFirstâ€Principlesâ€•kinetic monte carlo simulations revisited: CO oxidation over RuO₂(110). Journal of Computational Chemistry, 2012, 33, 757-766.	3.3	43
87	Oxidation of HCl over TiO₂-Supported RuO₂: A Density Functional Theory Study. Journal of Physical Chemistry C, 2010, 114, 22624-22629.	3.1	42
88	Crystals from metallic clusters: A first-principles calculation. Physical Review B, 1993, 48, 1981-1983.	3.2	39
89	Elemental Identification by Combining Atomic Force Microscopy and Kelvin Probe Force Microscopy. ACS Nano, 2018, 12, 5274-5283.	14.6	37
90	Nitrogen Doping of Amorphous Carbon Surfaces. Physical Review Letters, 1999, 83, 5346-5349.	7.8	36

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91	Understanding the Superior Stability of Singleâ€Molecule Magnets on an Oxide Film. Advanced Science, 2019, 6, 1901736.	11.2	36
92	Adsorption characteristics ofCOandN2onRuO2(110). Physical Review B, 2001, 63, .	3.2	35
93	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
94	Anomalous hydrogen adsorption sites found for the c(2Ã—2)-3H phases formed on the Re(101Ì„0) and Ru(101Ì„0) surfaces. Journal of Chemical Physics, 1998, 108, 8671-8679.	3.0	34
95	Adsorption of silicon on Au(110): An ordered two dimensional surface alloy. Applied Physics Letters, 2012, 101, .	3.3	34
96	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
97	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
98	Rocking-motion-induced charging ofC60onhâ^'BNâ^•Ni(111). Physical Review B, 2005, 71, .	3.2	33
99	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
100	Ionic Liquids from Carâ^'Parrinello Simulations, Part I:Â Liquid AlCl3. Journal of Physical Chemistry B, 2006, 110, 11475-11480.	2.6	31
101	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
102	Formation, migration, and clustering of point defects in CuInSe₂from first principles. Journal of Physics Condensed Matter, 2014, 26, 345501.	1.8	31
103	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
104	Structure of CAl12. Journal of Chemical Physics, 1995, 103, 8075-8080.	3.0	30
105	Introduction and recovery of point defects in electron-irradiated Te- and Si-doped GaAs studied by positron lifetime spectroscopy. Physical Review B, 1995, 52, 10932-10946.	3.2	30
106	Intimate interplay of theory and experiments in model catalysis. Surface Science, 2009, 603, 1717-1723.	1.9	30
107	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
108	Phosphorus vacancy in InP: A negative-Ucenter. Physical Review B, 1993, 47, 6381-6384.	3.2	29

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109	Carbon dioxide in silicate melts at upper mantle conditions: Insights from atomistic simulations. Chemical Geology, 2015, 418, 77-88.	3.3	29
110	First-principles simulation of collision cascades in Si to test pair-potentials for Si-Si interaction at 10 eVâ€“5 keV. Nuclear Instruments & Methods in Physics Research B, 1994, 88, 382-386.	1.4	28
111	Dynamic response of chlorine atoms on a RuO2(110) model catalyst surface. Physical Chemistry Chemical Physics, 2010, 12, 15358.	2.8	28
112	Dynamical Crossover at the Liquid-Liquid Transformation of a Compressed Molten Alkali Metal. Physical Review Letters, 2013, 111, 077801.	7.8	28
113	First-principles simulation of intrinsic collision cascades in KCl and NaCl to test interatomic potentials at energies between 5 and 350 eV. Physical Review Letters, 1991, 67, 3692-3695.	7.8	27
114	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></mm Anab initiostudy. Physical Review B, 2015, 92, .	3.2	27
115	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
116	Hydrogen-Promoted Chlorination of RuO₂(110). Journal of Physical Chemistry C, 2010, 114, 10901-10909.	3.1	25
117	Vacancies in CuInSe₂: new insights from hybrid-functional calculations. Journal of Physics Condensed Matter, 2011, 23, 422202.	1.8	25
118	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
119	Doping-induced reorientation ofC60molecules on Ag(111). Physical Review B, 2005, 72, .	3.2	23
120	LEED and DFT investigation on the (2Ã—2)-S overlayer on Co(0001). Surface Science, 2005, 599, 113-121.	1.9	22
121	Mass transport in CuInSe2 from first principles. Journal of Applied Physics, 2013, 113, .	2.5	22
122	Combined experiment and theory approach in surface chemistry: Stairway to heaven?. Surface Science, 2015, 640, 165-180.	1.9	22
123	Reaction mechanism of ammonia oxidation over RuO2(110): A combined theory/experiment approach. Surface Science, 2009, 603, L113-L116.	1.9	21
124	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
125	Kondo-effect of substitutional cobalt impurities at copper surfaces. New Journal of Physics, 2009, 11, 113015.	2.9	20
126	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

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127	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
128	Ordered phases of Na adsorbed on Pt(111):â€‚â€‚Experiment and theory. Physical Review B, 2001, 63, .	3.2	17
129	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
130	Photoelectron diffraction in the x-ray and ultraviolet regime: Sn-phthalocyanine on Ag(111). Physical Review B, 2013, 87, .	3.2	17
131	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
132	Large dispersion of incoherent spectral features in highly orderedC60chains. Physical Review B, 2006, 74, .	3.2	16
133	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
134	<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
135	Melting temperature of water: DFT-based molecular dynamics simulations with D3 dispersion correction. Physical Review B, 2016, 94, .	3.2	15
136	Strong3p-T1uhybridization inAr@C60. Physical Review A, 2010, 82, .	2.5	14
137	Tunable Interface of Ruthenium Porphyrins and Silver. Journal of Physical Chemistry C, 2021, 125, 3215-3224.	3.1	14
138	The adsorption structure on Co{0001}: a combined Tensor LEED and DFT study. Surface Science, 2004, 572, 1-10.	1.9	13
139	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
140	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
141	Combined ARPES and STM study of Pb/Au(111) MoirÃ© structure: One overlayer, two symmetries. Physical Review B, 2013, 87, .	3.2	13
142	Hierarchically Organized Bimolecular Ladder Network Exhibiting Guided One-Dimensional Diffusion. ACS Nano, 2012, 6, 549-556.	14.6	12
143	Bottom-Up Fabrication of a Metal-Supported Oxoâ€“Metal Porphyrin. Journal of Physical Chemistry C, 2019, 123, 31011-31025.	3.1	12
144	Conformational Control of Chemical Reactivity for Surfaceâ€Confined Ruâ€Porphyrins. Angewandte Chemie - International Edition, 2021, 60, 16561-16567.	13.8	12

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145	Magnetic 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:mi mathvariant="normal">C</mml:mi><mml:mn>80</mml:mn></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
146	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
147	Conformations of an aminoâ€“amidoâ€“thiolate self-assembled layer on gold in air and in electrolytes. Journal of Electroanalytical Chemistry, 2003, 550-551, 113-124.	3.8	10
148	Solvent effects on the vibrational spectrum of 3-hydroxyflavone. Journal of Molecular Liquids, 2019, 275, 723-728.	4.9	10
149	On the possible identification of defects using the autocorrelation function approach in double Doppler broadening of annihilation radiation spectroscopy. Journal of Physics Condensed Matter, 1998, 10, 10475-10492.	1.8	9
150	The thermodynamic stability and simulated STM images of graphene nanoribbons. Physica Status Solidi (B): Basic Research, 2009, 246, 2586-2591.	1.5	9
151	Extracting chemical information from plane wave calculations by a 3D â€˜fuzzy atomsâ€™ analysis. Chemical Physics Letters, 2013, 563, 97-101.	2.6	9
152	Chemical Reactions on Metal-supported Hexagonal Boron Nitride Investigated with Density Functional Theory. Chimia, 2014, 68, 596.	0.6	9
153	Charge-density correlations in pressurized liquid lithium calculated usingab initiomolecular dynamics. Physical Review B, 2014, 90, .	3.2	9
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