

Alessandro Fortunelli

List of Publications by Year in descending order

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298
papers

11,405
citations

34076

52
h-index

39638

94
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310
all docs

310
docs citations

310
times ranked

10096
citing authors

#	ARTICLE	IF	CITATIONS
1	Vertical Heterostructures between Transition-Metal Dichalcogenides: A Theoretical Analysis of the NbS ₂ /WSe ₂ Junction. <i>Advanced Electronic Materials</i> , 2022, 8, .	2.6	6
2	Reaction Mechanisms, Kinetics, and Improved Catalysts for Ammonia Synthesis from Hierarchical High Throughput Catalyst Design. <i>Accounts of Chemical Research</i> , 2022, 55, 1124-1134.	7.6	23
3	Ab Initio Modeling of the ZnO-Cu(111) Interface. <i>Journal of Physical Chemistry C</i> , 2022, 126, 764-771.	1.5	7
4	Plasmonic Circular Dichroism in Chiral Gold Nanowire Dimers. <i>Molecules</i> , 2022, 27, 93.	1.7	5
5	Exploring the materials space in the smallest particle size range: from heterogeneous catalysis to electrocatalysis and photocatalysis. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 12083-12115.	1.3	14
6	Adsorption and Activation of CO ₂ on a Au ₁₉ Pt Subnanometer Cluster in Aqueous Environment. <i>Computational and Theoretical Chemistry</i> , 2022, , 113701.	1.1	2
7	Unfolding the structural stability of nanoalloys via symmetry-constrained genetic algorithm and neural network potential. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	9
8	Experimental Sabatier plot for predictive design of active and stable Pt-alloy oxygen reduction reaction catalysts. <i>Nature Catalysis</i> , 2022, 5, 513-523.	16.1	57
9	Mechanisms of the Oxygen Evolution Reaction on NiFe ₂ O ₄ and CoFe ₂ O ₄ Inverse-Spinel Oxides. <i>ACS Catalysis</i> , 2022, 12, 9058-9073.	5.5	40
10	Pristine graphene covalent functionalization with aromatic aziridines and their application in the sensing of volatile amines – an <i>ab initio</i> investigation. <i>RSC Advances</i> , 2021, 11, 7070-7077.	1.7	10
11	An augmented (multi-descriptor) grouping algorithm to optimize chemical ordering in nanoalloys. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 23075-23089.	1.3	2
12	Theoretical Investigation of Photoinduced Processes in Subnanometer Oxide-Supported Metal Catalysts. <i>Journal of Physical Chemistry C</i> , 2021, 125, 2022-2032.	1.5	4
13	Diverse Phases of Carbonaceous Materials from Stochastic Simulations. <i>ACS Nano</i> , 2021, 15, 6369-6385.	7.3	10
14	Predictions of Chemical Shifts for Reactive Intermediates in CO ₂ Reduction under Operando Conditions. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 31554-31560.	4.0	12
15	Circularly Polarized Plasmons in Chiral Gold Nanowires via Quantum-Mechanical Design. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 5829-5835.	2.1	4
16	Understanding Reaction Networks through Controlled Approach to Equilibrium Experiments Using Transient Methods. <i>Journal of the American Chemical Society</i> , 2021, 143, 10998-11006.	6.6	6
17	6 The use of hydrogen in ammonia synthesis, and in oxygen and carbon dioxide catalytic reduction – the reaction mechanisms. , 2021, , 269-302.		0
18	Predictive optical photoabsorption of Ag ₂₄ Au(DMBT) ₁₈ via efficient TDDFT simulations. <i>Journal of Chemical Physics</i> , 2021, 155, 084103.	1.2	12

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19	Nanomolecular Metallurgy: Transformation from Au ₁₄₄ (SCH ₂ CH ₂ Ph) ₆₀ to Au ₂₇₉ (SPh- <i>i>t</i> /i>Bu) ₈₄ . Journal of Physical Chemistry C, 2021, 125, 20488-20502.	1.5	4
20	Discovering indium as hydrogen production booster for a Cu/SiO ₂ catalyst in steam reforming of methanol. Applied Catalysis B: Environmental, 2021, 297, 120398.	10.8	26
21	Design of a fluorescent and clickable Ag ₃₈ (SRN ₃) ₂₄ nanocluster platform: synthesis, modeling and self-assembling. Nanoscale Advances, 2021, 3, 2948-2960.	2.2	2
22	Controlling the Shapes of Nanoparticles by Dopant-Induced Enhancement of Chemisorption and Catalytic Activity: Application to Fe-Based Ammonia Synthesis. ACS Nano, 2021, 15, 1675-1684.	7.3	11
23	Optical Activity of Metal Nanoclusters Deposited on Regular and Doped Oxide Supports from First-Principles Simulations. Molecules, 2021, 26, 6961.	1.7	2
24	Density Functional Theory Investigation of Graphene Functionalization with Activated Carbenes and Its Application in the Sensing of Heavy Metallic Cations. Journal of Physical Chemistry C, 2021, 125, 26418-26428.	1.5	11
25	Vibrational Spectroscopy Signatures of Catalytically Relevant Configurations for N ₂ Reduction to NH ₃ on Fe Surfaces via Density Functional Theory. Journal of Physical Chemistry C, 2021, 125, 27919-27930.	1.5	1
26	Isomeric Thiolate Monolayer Protected Au ₉₂ and Au ₁₀₂ Nanomolecules. Journal of Physical Chemistry C, 2020, 124, 1655-1666.	1.5	9
27	Chiral Functionalization of an Atomically Precise Noble Metal Cluster: Insights into the Origin of Chirality and Photoluminescence. ACS Nano, 2020, 14, 9687-9700.	7.3	56
28	Discovery of Dramatically Improved Ammonia Synthesis Catalysts through Hierarchical High-Throughput Catalyst Screening of the Fe(211) Surface. Chemistry of Materials, 2020, 32, 9914-9924.	3.2	6
29	Theoretical Analysis of a 2D Metallic/Semiconducting Transition-Metal Dichalcogenide NbS ₂ /WSe ₂ Hybrid Interface. Advanced Theory and Simulations, 2020, 3, 2000164.	1.3	4
30	The Missing Link: Au ₁₉₁ (SPh-tBu) ₆₆ Janus Nanoparticle with Molecular and Bulk-Metal-like Properties. Journal of the American Chemical Society, 2020, 142, 15799-15814.	6.6	48
31	An efficient hybrid scheme for time dependent density functional theory. Journal of Chemical Physics, 2020, 152, 184104.	1.2	10
32	Si-Doped Fe Catalyst for Ammonia Synthesis at Dramatically Decreased Pressures and Temperatures. Journal of the American Chemical Society, 2020, 142, 8223-8232.	6.6	28
33	Edge Defects Promoted Oxidation of Monolayer WS ₂ Synthesized on Epitaxial Graphene. Journal of Physical Chemistry C, 2020, 124, 9035-9044.	1.5	22
34	Reactivity and Catalysis by Nanoalloys. , 2020, , 267-345.		2
35	Selectivity-Driven Design of the Ag-Cu Alloys for the Ethylene Epoxidation. Industrial & Engineering Chemistry Research, 2019, 58, 12996-13006.	1.8	5
36	Ultrathin WO ₃ Bilayer on Ag(100): A Model for the Structure of 2D WO ₃ Nanosheets. Journal of Physical Chemistry C, 2019, 123, 27584-27593.	1.5	11

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37	Optical Properties and Chemical Ordering of Ag@Pt Nanoparticles: A Computational Study. Journal of Physical Chemistry C, 2019, 123, 25482-25491.	1.5	11
38	Laser-Beam-Patterned Topological Insulating States on Thin Semiconducting MoS_2 . Physical Review Letters, 2019, 123, 146803.	2.9	23
39	Effect of Co doping on mechanism and kinetics of ammonia synthesis on Fe(111) surface. Journal of Catalysis, 2019, 370, 364-371.	3.1	13
40	Highly Efficient Ni-Doped Iron Catalyst for Ammonia Synthesis from Quantum-Mechanics-Based Hierarchical High-Throughput Catalyst Screening. Journal of Physical Chemistry C, 2019, 123, 17375-17383.	1.5	16
41	2D oxides on metal materials: concepts, status, and perspectives. Physical Chemistry Chemical Physics, 2019, 21, 11510-11536.	1.3	37
42	Reaction mechanism and kinetics for ammonia synthesis on the Fe(211) reconstructed surface. Physical Chemistry Chemical Physics, 2019, 21, 11444-11454.	1.3	27
43	Reaction intermediates during operando electrocatalysis identified from full solvent quantum mechanics molecular dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 7718-7722.	3.3	70
44	Phonon-assisted carrier transport through a lattice-mismatched interface. NPG Asia Materials, 2019, 11, .	3.8	5
45	Crystal Structure of Au _{36-x} Ag _x (SPh-t-Bu) ₂₄ Nanoparticle and the Role of Ag Doping in Excited State Coupling. Journal of Physical Chemistry C, 2019, 123, 29484-29494.	1.5	13
46	Ultralow Specific Contact Resistivity in Metal-Graphene Junctions via Contact Engineering. Advanced Materials Interfaces, 2019, 6, 1801285.	1.9	41
47	Pd doping, conformational, and charge effects on the dichroic response of a monolayer protected Au ₃₈ (SR) ₂₄ nanocluster. Physical Chemistry Chemical Physics, 2019, 21, 3585-3596.	1.3	6
48	Au ₂₇₉ (SR) ₈₄ : The Smallest Gold Thiolate Nanocrystal That Is Metallic and the Birth of Plasmon. Journal of Physical Chemistry Letters, 2018, 9, 1295-1300.	2.1	65
49	Principles of Optical Spectroscopy of Aromatic Alloy Nanomolecules: Au ₃₆ @Ag _x (SPh-t-Bu) ₂₄ . Journal of Physical Chemistry C, 2018, 122, 4524-4531.	1.5	28
50	Bimetallic Ag@Pt Subnanometer Supported Clusters as Highly Efficient and Robust Oxidation Catalysts. Angewandte Chemie, 2018, 130, 1223-1227.	1.6	3
51	Reaction Mechanism and Kinetics for Ammonia Synthesis on the Fe(111) Surface. Journal of the American Chemical Society, 2018, 140, 6288-6297.	6.6	126
52	Perspective: Size selected clusters for catalysis and electrochemistry. Journal of Chemical Physics, 2018, 148, 110901.	1.2	93
53	Empirical-potential global minima and DFT local minima of trimetallic Ag Au Pt (l+m+n= 13, 19, 33, 38) clusters. Computational Materials Science, 2018, 141, 30-40.	1.4	29
54	Bimetallic Ag@Pt Subnanometer Supported Clusters as Highly Efficient and Robust Oxidation Catalysts. Angewandte Chemie - International Edition, 2018, 57, 1209-1213.	7.2	47

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55	Atomically precise Au ₁₄₄ (SR) ₆₀ nanoclusters (R = Et, Pr) are capped by 12 distinct ligand types of 5-fold equivalence and display gigantic diastereotopic effects. <i>Chemical Science</i> , 2018, 9, 8796-8805.	3.7	30
56	QM-Mechanism-Based Hierarchical High-Throughput in Silico Screening Catalyst Design for Ammonia Synthesis. <i>Journal of the American Chemical Society</i> , 2018, 140, 17702-17710.	6.6	32
57	Electronic Structure of Oxide Ultrathin Layers on Metal Surfaces. , 2018, , 86-96.		0
58	TDDFT Study of the Optical Spectra of Free and Supported Binary Coinage Metal Hexamers: Effect of Doping and Support. <i>Journal of Physical Chemistry C</i> , 2018, 122, 23143-23152.	1.5	5
59	Chirality in bare and ligand-protected metal nanoclusters. <i>Advances in Physics: X</i> , 2018, 3, 1509727.	1.5	21
60	Stacking and interlayer electron transport in MoS_2 . <i>Physical Review B</i> , 2018, 98, .		
61	Time-dependent density functional study of the photoabsorption spectrum of Au ₂₅ (SC ₂ H ₄ C ₆ H ₅) ₁₈ anion: Validation of the computational protocol. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25769.	1.0	9
62	Au ₃₆ (SePh) ₂₄ nanomolecules: synthesis, optical spectroscopy and theoretical analysis. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 13255-13262.	1.3	10
63	Ligand Structure Determines Nanoparticles' Atomic Structure, Metal-Ligand Interface and Properties. <i>Frontiers in Chemistry</i> , 2018, 6, 330.	1.8	58
64	Hydrogen evolution reaction (HER) on Au@Ag ultrananoclusters as electro-catalysts. <i>Nanoscale</i> , 2018, 10, 17730-17737.	2.8	21
65	Individual Component Map of Rotatory Strength and Rotatory Strength Density Plots As Analysis Tools of Circular Dichroism Spectra of Complex Systems. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3703-3714.	2.3	13
66	Optical Properties of Metal Nanoclusters Theory. , 2018, , 534-545.		4
67	High-Performance 2D p-Type Transistors Based on GaSe Layers: An Ab Initio Study. <i>Advanced Electronic Materials</i> , 2017, 3, 1600399.	2.6	20
68	Alumina-supported sub-nanometer Pt ₁₀ clusters: amorphization and role of the support material in a highly active CO oxidation catalyst. <i>Journal of Materials Chemistry A</i> , 2017, 5, 4923-4931.	5.2	72
69	Ligand-Enhanced Optical Response of Gold Nanomolecules and Its Fragment Projection Analysis: The Case of Au ₃₀ (SR) ₁₈ . <i>Journal of Physical Chemistry C</i> , 2017, 121, 10832-10842.	1.5	21
70	Au ₂₁ S(SAdm) ₁₅ : Crystal Structure, Mass Spectrometry, Optical Spectroscopy, and First-Principles Theoretical Analysis. <i>Journal of Physical Chemistry C</i> , 2017, 121, 10865-10869.	1.5	29
71	Growth-Induced Strain in Chemical Vapor Deposited Monolayer MoS ₂ : Experimental and Theoretical Investigation. <i>Advanced Materials Interfaces</i> , 2017, 4, 1700031.	1.9	50
72	Magnetic Ordering in Gold Nanoclusters. <i>ACS Omega</i> , 2017, 2, 2607-2617.	1.6	69

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73	Au ₃₈ (SPh) ₂₄ : Au ₃₈ Protected with Aromatic Thiolate Ligands. Journal of Physical Chemistry Letters, 2017, 8, 1530-1537.	2.1	33
74	Au ₂₁ S(SAdm) ₁₅ : An Anisotropic Gold Nanomolecule. Optical and Photoluminescence Spectroscopy and First-Principles Theoretical Analysis. Journal of Physical Chemistry Letters, 2017, 8, 457-462.	2.1	8
75	Intense fluorescence of Au ₂₀ . Journal of Chemical Physics, 2017, 147, 074301.	1.2	18
76	Core-Size Conversion of Au ₃₈ (SCH ₂ CH ₂ Ph) ₂₄ to Au ₃₀ (S <i>t</i> Bu) ₁₈ Nanomolecules. Journal of Physical Chemistry C, 2017, 121, 14929-14935.	1.5	22
77	Electrical properties of graphene-metal contacts. Scientific Reports, 2017, 7, 5109.	1.6	119
78	Transistor Concepts Based on Lateral Heterostructures of Metallic and Semiconducting Phases of MoS_2 Physical Review Applied, 2017, 8, .	1.5	38
79	Core Size Interconversions of Au ₃₀ (S <i>t</i> Bu) ₁₈ and Au ₃₆ (SPhX) ₂₄ . Journal of Physical Chemistry C, 2017, 121, 14914-14919.	1.5	38
80	A new time-dependent density functional method for molecular plasmonics: Formalism, implementation, and the Au ₁₄₄ (SH) ₆₀ case study. International Journal of Quantum Chemistry, 2016, 116, 1603-1611.	1.0	24
81	Nanoscale Domain Structure and Defects in a 2-D WO ₃ Layer on Pd(100). Journal of Physical Chemistry C, 2016, 120, 28682-28693.	1.5	21
82	Optical absorption of (Ag-Au) ₁₃₃ (SCH ₃) ₅₂ bimetallic monolayer-protected clusters. Progress in Natural Science: Materials International, 2016, 26, 467-476.	1.8	2
83	Two-dimensional transistors based on MoS ₂ lateral heterostructures. , 2016, , .		2
84	Photoabsorption of Icosahedral Noble Metal Clusters: An Efficient TDDFT Approach to Large-Scale Systems. Journal of Physical Chemistry C, 2016, 120, 12773-12782.	1.5	57
85	Atomistic and Electronic Structure Methods for Nanostructured Oxide Interfaces. Springer Series in Materials Science, 2016, , 39-90.	0.4	4
86	Oxide Materials at the Two-Dimensional Limit. Springer Series in Materials Science, 2016, , .	0.4	24
87	Gate-Tunable Atomically Thin Lateral MoS ₂ Schottky Junction Patterned by Electron Beam. Nano Letters, 2016, 16, 3788-3794.	4.5	99
88	Extension of the Time-Dependent Density Functional Complex Polarizability Algorithm to Circular Dichroism: Implementation and Applications to Ag ₈ and Au ₃₈ (SCH ₂ CH ₂ Ph) ₂₄ . Journal of Physical Chemistry C, 2016, 120, 24335-24345.	1.5	14
89	Editorial: Nanocatalysis. Catalysis Science and Technology, 2016, 6, 6763-6765.	2.1	5
90	Ultrafine jagged platinum nanowires enable ultrahigh mass activity for the oxygen reduction reaction. Science, 2016, 354, 1414-1419.	6.0	1,292

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91	All-atom molecular dynamics simulations of multiphase segregated polyurea under quasistatic, adiabatic, uniaxial compression. <i>Polymer</i> , 2016, 106, 100-108.	1.8	16
92	Catalytic activity of Pt ₃₈ in the oxygen reduction reaction from first-principles simulations. <i>Catalysis Science and Technology</i> , 2016, 6, 6901-6909.	2.1	23
93	The quantum mechanics derived atomistic mechanism underlying the acceleration of catalytic CO oxidation on Pt(110) by surface acoustic waves. <i>Journal of Materials Chemistry A</i> , 2016, 4, 12036-12045.	5.2	7
94	Two-dimensional iron oxide bi-and trilayer structures on Pd(100). <i>Surface Science</i> , 2016, 645, 13-22.	0.8	10
95	Two-Dimensional Iron Tungstate: A Ternary Oxide Layer With Honeycomb Geometry. <i>Journal of Physical Chemistry C</i> , 2016, 120, 7629-7638.	1.5	28
96	Lattice Strain Defects in a Ceria Nanolayer. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1303-1309.	2.1	17
97	Crystal Structure and Theoretical Analysis of Green Gold Au ₃₀ (S-t-Bu) ₁₈ Nanomolecules and Their Relation to Au ₃₀ S(S-t-Bu) ₁₈ . <i>Journal of Physical Chemistry C</i> , 2016, 120, 6256-6261.	1.5	72
98	Nanoalloy Simulation. , 2016, , 2293-2305.		1
99	Simulation of Supported Metal Clusters. , 2016, , 3680-3692.		0
100	Does enhanced oxygen activation always facilitate CO oxidation on gold clusters?. <i>Journal of Computational Chemistry</i> , 2015, 36, 2177-2187.	1.5	10
101	Designing ligand-enhanced optical absorption of thiolated gold nanoclusters. <i>Chemical Communications</i> , 2015, 51, 7935-7938.	2.2	31
102	Transformation of Au ₁₄₄ (SCH ₂ CH ₂ Ph) ₆₀ to Au ₁₃₃ (SPh-t-Bu) ₅₂ Nanomolecules: Theoretical and Experimental Study. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 2134-2139.	2.1	58
103	Au ₁₃₃ (SPh-t-Bu) ₅₂ Nanomolecules: X-ray Crystallography, Optical, Electrochemical, and Theoretical Analysis. <i>Journal of the American Chemical Society</i> , 2015, 137, 4610-4613.	6.6	265
104	Understanding the nature of metal-graphene contacts: A theoretical and experimental study. , 2015, , .		3
105	Analogy between homogeneous and heterogeneous catalysis by subnanometer metal clusters: Ethylene oxidation on Ag trimers supported on MgO(1 0 0). <i>Inorganica Chimica Acta</i> , 2015, 431, 150-155.	1.2	11
106	Optimizing the oxygen evolution reaction for electrochemical water oxidation by tuning solvent properties. <i>Nanoscale</i> , 2015, 7, 4514-4521.	2.8	20
107	The atomistic origin of the extraordinary oxygen reduction activity of Pt ₃ Ni ₇ fuel cell catalysts. <i>Chemical Science</i> , 2015, 6, 3915-3925.	3.7	53
108	Chemical properties of two-dimensional oxide systems: Adsorption of (WO ₃) ₃ clusters on CuWO ₄ . <i>Surface Science</i> , 2015, 640, 96-103.	0.8	9

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109	Temperature and Doping Effect on Thermal Conductivity of Copper–Gold Icosahedral Bimetallic Nanoclusters and Bulk Structures. <i>Journal of Physical Chemistry C</i> , 2015, 119, 7922-7932.	1.5	14
110	Optical properties of nanoalloys. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 27952-27967.	1.3	45
111	Organosoluble Au ₁₀₂ (SPh) ₄₄ Nanomolecules: Synthesis, Isolation, Compositional Assignment, Core Conversion, Optical Spectroscopy, Electrochemistry, and Theoretical Analysis. <i>Journal of Physical Chemistry C</i> , 2015, 119, 25077-25084.	1.5	24
112	Exploring the energy landscape of Pt Au ₁₁₅ nanoalloys. <i>Computational and Theoretical Chemistry</i> , 2015, 1074, 150-156.	1.1	4
113	Comment on “Au–Ag ₁₄₄ (SR) ₆₀ alloy nanomolecules” by C. Kumara and A. Dass, <i>Nanoscale</i> , 2011, 3, 3064. <i>Nanoscale</i> , 2015, 7, 8166-8167.	2.8	17
114	Simulation of Supported Metal Clusters. , 2015, , 1-14.		1
115	Nanoalloy Simulation. , 2015, , 1-13.		0
116	Ligand/cluster/support catalytic complexes in heterogeneous ultrananocatalysis: NO oxidation on Ag ₃ /MgO(100). <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26570-26577.	1.3	10
117	Concepts in theoretical heterogeneous ultrananocatalysis. <i>Comptes Rendus Chimie</i> , 2014, 17, 625-633.	0.2	26
118	Tuning the catalytic activity of Au–Pd nanoalloys in CO oxidation via composition. <i>Journal of Catalysis</i> , 2014, 314, 47-55.	3.1	33
119	Dramatic Increase in the Oxygen Reduction Reaction for Platinum Cathodes from Tuning the Solvent Dielectric Constant. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 6669-6672.	7.2	33
120	Metal Tungstates at the Ultimate Two-Dimensional Limit: Fabrication of a CuWO ₄ Nanophase. <i>ACS Nano</i> , 2014, 8, 3947-3954.	7.3	53
121	Au ₂₄ (SAdm) ₁₆ Nanomolecules: X-ray Crystal Structure, Theoretical Analysis, Adaptability of Adamantane Ligands to Form Au ₂₃ (SAdm) ₁₆ and Au ₂₅ (SAdm) ₁₆ , and Its Relation to Au ₂₅ (SR) ₁₈ . <i>Journal of the American Chemical Society</i> , 2014, 136, 14933-14940.	6.6	139
122	Optical Properties of Pt and Ag–Pt Nanoclusters from TDDFT Calculations: Plasmon Suppression by Pt Poisoning. <i>Journal of Physical Chemistry C</i> , 2014, 118, 28101-28108.	1.5	18
123	Probing the atomic structure of metallic nanoclusters with the tip of a scanning tunneling microscope. <i>Nanoscale</i> , 2014, 6, 2170-2176.	2.8	20
124	Optical Properties of Silver Nanoshells from Time-Dependent Density Functional Theory Calculations. <i>Journal of Physical Chemistry C</i> , 2014, 118, 12450-12458.	1.5	38
125	A grouping approach to homotop global optimization in alloy nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 24256-24265.	1.3	34
126	Composition-dependent melting behaviour of Na _x K _{55-x} core–shell nanoalloys. <i>Molecular Physics</i> , 2014, 112, 2933-2944.	0.8	2

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127	Experimental and Theoretical Scanning Tunneling Spectroscopy Analysis of an Ultrathin Titania Film and Adsorbed Au Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2014, 118, 14640-14646.	1.5	2
128	Redox processes at a nanostructured interface under strong electric fields. <i>Nanoscale</i> , 2014, 6, 10589-10595.	2.8	4
129	Atomistic Quantum Plasmonics of Gold Nanowire Arrays. <i>ACS Photonics</i> , 2014, 1, 315-322.	3.2	13
130	Communication: Striking dependence of diffusion kinetics in Ag-Cu nanoalloys upon composition and quantum effects. <i>Journal of Chemical Physics</i> , 2014, 141, 041108.	1.2	10
131	Influence of temperature and H ₂ adsorption on the structure of silica-supported gold subnanometer clusters. <i>Computational and Theoretical Chemistry</i> , 2013, 1021, 222-228.	1.1	10
132	Reactivity and catalysis by nanoalloys. , 2013, , 283-344.		1
133	Structure and Electronic Properties of CoO Nanostructures on a Vicinal Pd(100) Surface. <i>Journal of Physical Chemistry C</i> , 2013, 117, 18464-18474.	1.5	12
134	Effect of CO and H adsorption on the compositional structure of binary nanoalloys via DFT modeling. <i>European Physical Journal D</i> , 2013, 67, 1.	0.6	13
135	Electronic excited states at ultrathin dielectric-metal interfaces. <i>Physical Review B</i> , 2013, 88, .	1.1	5
136	Alloys on the Nanoscale. , 2013, , 409-472.		1
137	Global Minimum Pt ₁₃ M ₂₀ (M = Ag, Au, Cu, Pd) Dodecahedral Core-Shell Clusters. <i>Journal of Physical Chemistry A</i> , 2013, 117, 14261-14266.	1.1	32
138	Study of two dimensional anisotropic Ising models via a renormalization group approach. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2013, 392, 5604-5614.	1.2	3
139	Communication: Kinetics of chemical ordering in Ag-Au and Ag-Ni nanoalloys. <i>Journal of Chemical Physics</i> , 2013, 139, 111102.	1.2	29
140	Direct atomic imaging and density functional theory study of the Au ₂₄ Pd ₁ cluster catalyst. <i>Nanoscale</i> , 2013, 5, 9620.	2.8	37
141	DFT study of the structures and energetics of 98-atom AuPd clusters. <i>Nanoscale</i> , 2013, 5, 646-652.	2.8	56
142	Adsorption-Induced Restructuring and Early Stages of Carbon-Nanotube Growth on Ni Nanoparticles. <i>Chemistry - A European Journal</i> , 2013, 19, 406-413.	1.7	2
143	Nanostripe Pattern of NaCl Layers on Cu(110). <i>Physical Review Letters</i> , 2013, 110, 216101.	2.9	18
144	Density-Functional Theory of Free and Supported Metal Nanoclusters and Nanoalloys. <i>Nanostructure Science and Technology</i> , 2013, , 29-79.	0.1	7

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145	Modelling the metal-on-top effect for Pd clusters on the MgO{100} substrate. <i>Journal of Chemical Physics</i> , 2013, 138, 224703.	1.2	11
146	Computational Approaches to the Chemical Conversion of Carbon Dioxide. <i>ChemSusChem</i> , 2013, 6, 944-965.	3.6	144
147	Structure-Property Relationship and Chemical Aspects of Oxide-Metal Hybrid Nanostructures. <i>Chemical Reviews</i> , 2013, 113, 4314-4372.	23.0	160
148	Structural Motifs of Bimetallic Pt ₁₀₁ -Au Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2013, 117, 20967-20974.	1.5	12
149	Kinetic asymmetry in the growth of two-dimensional Mn oxide nanostripes. <i>Physical Review B</i> , 2013, 88, .	1.1	14
150	Ordered Arrays of Size-Selected Oxide Nanoparticles. <i>Physical Review Letters</i> , 2012, 108, 195507.	2.9	21
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