Alessandro Fortunelli

List of Publications by Year
in descending order

298 papers	11,405 citations	34105 52 h-index	39675 94 g-index
310 all docs	310 docs citations	310 times ranked	10096 citing authors

#	Article	IF	Citations
1	Ultrafine jagged platinum nanowires enable ultrahigh mass activity for the oxygen reduction reaction. Science, 2016, 354, 1414-1419.	12.6	1,292
2	Crossover among structural motifs in transition and noble-metal clusters. Journal of Chemical Physics, 2002, 116, 3856-3863.	3.0	431
3	Magic Polyicosahedral Core-Shell Clusters. Physical Review Letters, 2004, 93, 105503.	7.8	361
4	Global optimization of bimetallic cluster structures. I. Size-mismatched Agâ€“Cu, Agâ€“Ni, and Auâ€“Cu systems. Journal of Chemical Physics, 2005, 122, 194308.	3.0	307
5	Au₁₃₃(SPh-tBu)₅₂ Nanomolecules: X-ray Crystallography, Optical, Electrochemical, and Theoretical Analysis. Journal of the American Chemical Society, 2015, 137, 4610-4613.	13.7	265
6	Global optimization of bimetallic cluster structures. II. Size-matched Ag-Pd, Ag-Au, and Pd-Pt systems. Journal of Chemical Physics, 2005, 122, 194309.	3.0	192
7	Searching for the optimum structures of alloy nanoclusters. Physical Chemistry Chemical Physics, 2008, 10, 640-649.	2.8	185
8	Quantum effects on the structure of pure and binary metallic nanoclusters. Physical Review B, 2005, 72, .	3.2	174
9	Structureâ€“Property Relationship and Chemical Aspects of Oxideâ€“Metal Hybrid Nanostructures. Chemical Reviews, 2013, 113, 4314-4372.	47.7	160
10	Growth and Surface Structure of Zinc Oxide Layers on a Pd(111) Surface. Journal of Physical Chemistry C, 2010, 114, 15432-15439.	3.1	153
11	Theoretical Studies of Palladiumâ^'Gold Nanoclusters: Pdâ^'Au Clusters with up to 50 Atoms. Journal of Physical Chemistry C, 2009, 113, 9141-9152.	3.1	152
12	Structural motifs, mixing, and segregation effects in 38-atom binary clusters. Journal of Chemical Physics, 2008, 128, 134517.	3.0	147
13	Computational Approaches to the Chemical Conversion of Carbon Dioxide. ChemSusChem, 2013, 6, 944-965.	6.8	144
14	Au₂₄(SAdm)₁₆ Nanomolecules: X-ray Crystal Structure, Theoretical Analysis, Adaptability of Adamantane Ligands to Form Au₂₃(SAdm)₁₆ and Au₂₅(SAdm)₁₆, and Its Relation to Au₂₅(SR)₁₈. Journal of the American Chemical Society, 2014, 136, 14933-14940.	13.7	139
15	Validation of selfâ€consistent hybrid density functionals for the study of structural and electronic characteristics of organic Ï€ radicals. Journal of Chemical Physics, 1995, 102, 384-393.	3.0	138
16	Reaction Mechanism and Kinetics for Ammonia Synthesis on the Fe(111) Surface. Journal of the American Chemical Society, 2018, 140, 6288-6297.	13.7	126
17	Electrical properties of graphene-metal contacts. Scientific Reports, 2017, 7, 5109.	3.3	119
18	Size-dependent selectivity and activity of silver nanoclusters in the partial oxidation of propylene to propylene oxide and acrolein: A joint experimental and theoretical study. Catalysis Today, 2011, 160, 116-130.	4.4	115

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19	The Interaction of Coinage Metal Clusters with the MgO(100) Surface. Journal of Chemical Theory and Computation, 2005, 1, 972-985.	5.3	114
20	Amorphization Mechanism of Icosahedral Metal Nanoclusters. Physical Review Letters, 2004, 93, 065502.	7.8	113
21	Density-functional global optimization of gold nanoclusters. Physical Review B, 2006, 73, .	3.2	106
22	Optical Properties of Au Nanoclusters from TD-DFT Calculations. Journal of Physical Chemistry C, 2011, 115, 6277-6282.	3.1	100
23	Gate-Tunable Atomically Thin Lateral MoS₂ Schottky Junction Patterned by Electron Beam. Nano Letters, 2016, 16, 3788-3794.	9.1	99
24	Density-Functional Calculations on Platinum Nanoclusters:â€‰ Pt13, Pt38, and Pt55. Journal of Physical Chemistry A, 2003, 107, 2934-2942.	2.5	96
25	Patchy Multishell Segregation in Pdâ^'Pt Alloy Nanoparticles. Nano Letters, 2011, 11, 1766-1769.	9.1	94
26	Perspective: Size selected clusters for catalysis and electrochemistry. Journal of Chemical Physics, 2018, 148, 110901.	3.0	93
27	Electronic and Structural Shell Closure in AgCu and AuCu Nanoclusters. Journal of Physical Chemistry B, 2006, 110, 23197-23203.	2.6	90
28	A Mixed Structural Motif in 34-Atom Pdâ^'Pt Clusters. Journal of Physical Chemistry C, 2007, 111, 2936-2941.	3.1	90
29	Structures and energetics of 98 atom Pdâ€“Pt nanoalloys: potential stability of the Leary tetrahedron for bimetallic nanoparticles. Physical Chemistry Chemical Physics, 2007, 9, 5202.	2.8	84
30	The implementation of density functional theory within the polarizable continuum model for solvation. Chemical Physics Letters, 1994, 231, 34-39.	2.6	81
31	Correlation correction to the Hartree-Fock total energy of solids. Physical Review B, 1987, 36, 891-897.	3.2	75
32	Preparation, characterisation and structure of Ti and Al ultrathin oxide films on metals. International Reviews in Physical Chemistry, 2009, 28, 517-576.	2.3	75
33	Structures of metal nanoparticles adsorbed on MgO(001). I. Ag and Au. Journal of Chemical Physics, 2009, 130, 174702.	3.0	75
34	Crystal Structure and Theoretical Analysis of Green Gold Au₃₀(S-tBu)₁₈ Nanomolecules and Their Relation to Au₃₀S(S-tBu)₁₈. Journal of Physical Chemistry C, 2016, 120, 6256-6261.	3.1	72
35	Alumina-supported sub-nanometer Pt₁₀ clusters: amorphization and role of the support material in a highly active CO oxidation catalyst. Journal of Materials Chemistry A, 2017, 5, 4923-4931.	10.3	72
36	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.	7.1	70

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37	Magnetic Ordering in Gold Nanoclusters. ACS Omega, 2017, 2, 2607-2617.	3.5	69
38	Homogeneous Nucleation of Graphitic Nanostructures from Carbon Chains on Ni(111). Journal of Physical Chemistry C, 2011, 115, 10537-10543.	3.1	68
39	Au₂₇₉(SR)₈₄: The Smallest Gold Thiolate Nanocrystal That Is Metallic and the Birth of Plasmon. Journal of Physical Chemistry Letters, 2018, 9, 1295-1300.	4.6	65
40	Structure and diffusion of small Ag and Au clusters on the regular MgO (100) surface. New Journal of Physics, 2007, 9, 22-22.	2.9	64
41	Structure of Reduced Ultrathin TiO_x Polar Films on Pt(111). Journal of Physical Chemistry C, 2009, 113, 5721-5729.	3.1	64
42	Diffusion of Palladium Clusters on Magnesium Oxide. Physical Review Letters, 2005, 95, 246103.	7.8	62
43	Alloying Effects on the Optical Properties of Agâ€“Au Nanoclusters from TDDFT Calculations. Journal of Physical Chemistry C, 2011, 115, 24085-24091.	3.1	61
44	A Magic Pdâ‚Ag Binary Cluster on the Fs-Defected MgO(100) Surface. Journal of Physical Chemistry C, 2007, 111, 11384-11389.	3.1	60
45	Interface-Stabilized Phases of Metal-on-Oxide Nanodots. ACS Nano, 2008, 2, 1849-1856.	14.6	58
46	Transformation of Au₁₄₄(SCH₂CH₂Ph)₆₀ to Au₁₃₃(SPh-tBu)₅₂ Nanomolecules: Theoretical and Experimental Study. Journal of Physical Chemistry Letters, 2015, 6, 2134-2139.	4.6	58
47	Ligand Structure Determines Nanoparticles' Atomic Structure, Metal-Ligand Interface and Properties. Frontiers in Chemistry, 2018, 6, 330.	3.6	58
48	CO Oxidation by Subnanometer Ag_xAu_{3â€“x} Supported Clusters via Density Functional Theory Simulations. ACS Catalysis, 2012, 2, 1860-1864.	11.2	57
49	Photoabsorption of Icosahedral Noble Metal Clusters: An Efficient TDDFT Approach to Large-Scale Systems. Journal of Physical Chemistry C, 2016, 120, 12773-12782.	3.1	57
50	Experimental Sabatier plot for predictive design of active and stable Pt-alloy oxygen reduction reaction catalysts. Nature Catalysis, 2022, 5, 513-523.	34.4	57
51	DFT study of the structures and energetics of 98-atom AuPd clusters. Nanoscale, 2013, 5, 646-652.	5.6	56
52	Chiral Functionalization of an Atomically Precise Noble Metal Cluster: Insights into the Origin of Chirality and Photoluminescence. ACS Nano, 2020, 14, 9687-9700.	14.6	56
53	Optimization of chemical ordering in AgAu nanoalloys. Physical Chemistry Chemical Physics, 2011, 13, 10232.	2.8	55
54	Metal Tungstates at the Ultimate Two-Dimensional Limit: Fabrication of a CuWO₄ Nanophase. ACS Nano, 2014, 8, 3947-3954.	14.6	53

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55	The atomistic origin of the extraordinary oxygen reduction activity of Pt₃Ni₇fuel cell catalysts. Chemical Science, 2015, 6, 3915-3925.	7.4	53
56	Growthâ€Induced Strain in Chemical Vapor Deposited Monolayer MoS₂: Experimental and Theoretical Investigation. Advanced Materials Interfaces, 2017, 4, 1700031.	3.7	50
57	Oxidant-Induced Hydride Abstraction from [Pt(Î¼-PBut2)(H)(PBut2H)]2Yielding [Pt2(Î¼-PBut2)2(H)(PBut2H)2]C3(CN)5. Spectroscopic, Crystallographic, and Theoretical Comparison of the Structures of Two â€œTautomersâ€. Journal of the American Chemical Society, 1998, 120, 9564-9573.	13.7	49
58	Structural and electronic properties of Pt/Fe nanoclusters from EHT calculations. Computational and Theoretical Chemistry, 1999, 487, 251-266.	1.5	48
59	Density-functional study of Pt 13 and Pt 55 cuboctahedral clusters. Computational and Theoretical Chemistry, 2000, 501-502, 251-259.	1.5	48
60	Structures of metal nanoparticles adsorbed on MgO(001). II. Pt and Pd. Journal of Chemical Physics, 2009, 130, 174703.	3.0	48
61	The Missing Link: Au191(SPh-tBu)66 Janus Nanoparticle with Molecular and Bulk-Metal-like Properties. Journal of the American Chemical Society, 2020, 142, 15799-15814.	13.7	48
62	Validation of density-functional versus density-functional+U approaches for oxide ultrathin films. Journal of Chemical Physics, 2010, 132, 124703.	3.0	47
63	The Effect of CO and H Chemisorption on the Chemical Ordering of Bimetallic Clusters. Journal of Physical Chemistry C, 2010, 114, 19678-19686.	3.1	47
64	A first-principles theoretical approach to heterogeneous nanocatalysis. Nanoscale, 2012, 4, 1208-1219.	5.6	47
65	Bimetallic Agâ€Pt Subâ€nanometer Supported Clusters as Highly Efficient and Robust Oxidation Catalysts. Angewandte Chemie - International Edition, 2018, 57, 1209-1213.	13.8	47
66	Structure of Ag Clusters Grown on Fs-Defect Sites of an MgO(1â€‰0â€‰0) Surface. Chemistry - A European Journal, 2007, 13, 6408-6418.	3.3	46
67	Structure of a TiOx Zigzag-Like Monolayer on Pt(111). Journal of Physical Chemistry C, 2007, 111, 6095-6102.	3.1	45
68	Optical properties of nanoalloys. Physical Chemistry Chemical Physics, 2015, 17, 27952-27967.	2.8	45
69	Ab initio estimate of Hubbard model parameters:mA simple procedure appliedto BEDT-TTF salts. Physical Review B, 1997, 55, 16088-16095.	3.2	44
70	Density functional calculations on small platinum clusters: Pt n q (n =1â€“4, q =0,Â±1). Computational and Theoretical Chemistry, 1999, 493, 233-240.	1.5	44
71	Structures of gas-phase Agâ€“Pd nanoclusters: A computational study. Journal of Chemical Physics, 2010, 132, 234703.	3.0	44
72	Defect evolution in oxide nanophases: The case of a zigzag-like<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mi>x</mml:mi></mml:msub></mml:mrow></mml:math>phase on Pt(111). Physical Review B, 2008, 77, .	3.2	43

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73	Exotic Supported CoPt Nanostructures: From Clusters to Wires. Journal of Physical Chemistry Letters, 2010, 1, 111-115.	4.6	41
74	Ultralow Specific Contact Resistivity in Metalâ€“Graphene Junctions via Contact Engineering. Advanced Materials Interfaces, 2019, 6, 1801285.	3.7	41
75	Mechanisms of the Oxygen Evolution Reaction on NiFe₂O₄ and CoFe₂O₄ Inverse-Spinel Oxides. ACS Catalysis, 2022, 12, 9058-9073.	11.2	40
76	Epitaxy, Truncations, and Overhangs in Palladium Nanoclusters Adsorbed on MgO(001). Physical Review Letters, 2007, 98, 156101.	7.8	38
77	Template-assisted assembly of transition metal nanoparticles on oxide ultrathin films. Progress in Surface Science, 2011, 86, 59-81.	8.3	38
78	Optical Properties of Silver Nanoshells from Time-Dependent Density Functional Theory Calculations. Journal of Physical Chemistry C, 2014, 118, 12450-12458.	3.1	38
79	Transistor Concepts Based on Lateral Heterostructures of Metallic and Semiconducting Phases of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>MoS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow> Physical Review Applied, 2017, 8, .	3.8	38
80	Core Size Interconversions of Au₃₀(S-tBu)₁₈ and Au₃₆(SPhX)₂₄. Journal of Physical Chemistry C, 2017, 121, 14914-14919.	3.1	38
81	Chemisorption of CO and H on Pd, Pt and Au nanoclusters: a DFT approach. European Physical Journal D, 2009, 52, 131-134.	1.3	37
82	Direct atomic imaging and density functional theory study of the Au24Pd1 cluster catalyst. Nanoscale, 2013, 5, 9620.	5.6	37
83	2D oxides on metal materials: concepts, status, and perspectives. Physical Chemistry Chemical Physics, 2019, 21, 11510-11536.	2.8	37
84	Simulations of Lipid Adsorption on TiO₂ Surfaces in Solution. Langmuir, 2008, 24, 10145-10154.	3.5	35
85	Au<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>N</mml:mi></mml:msub></mml:math>clusters (<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML") Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 262 Td (display="in on MgO(100) surfaces: Effect of exact exchange and dispersion interactions on adhesion energies. Physical Review B, 2012, 85, .	3.2	35
86	Surface-Supported Gold Cages. Physical Review Letters, 2009, 102, 216102.	7.8	34
87	A grouping approach to homotop global optimization in alloy nanoparticles. Physical Chemistry Chemical Physics, 2014, 16, 24256-24265.	2.8	34
88	Tuning the catalytic activity of Auâ€“Pd nanoalloys in CO oxidation via composition. Journal of Catalysis, 2014, 314, 47-55.	6.2	33
89	Dramatic Increase in the Oxygen Reduction Reaction for Platinum Cathodes from Tuning the Solvent Dielectric Constant. Angewandte Chemie - International Edition, 2014, 53, 6669-6672.	13.8	33
90	Au₃₈(SPh)₂₄: Au₃₈ Protected with Aromatic Thiolate Ligands. Journal of Physical Chemistry Letters, 2017, 8, 1530-1537.	4.6	33

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91	An SCF technique for excited states. Theoretica Chimica Acta, 1987, 71, 467-478.	0.8	32
92	Global Minimum Pt₁₃M₂₀ (M = Ag, Au, Cu, Pd) Dodecahedral Coreâ€“Shell Clusters. Journal of Physical Chemistry A, 2013, 117, 14261-14266.	2.5	32
93	QM-Mechanism-Based Hierarchical High-Throughput in Silico Screening Catalyst Design for Ammonia Synthesis. Journal of the American Chemical Society, 2018, 140, 17702-17710.	13.7	32
94	Correlation correction to the Hartree-Fock total energy of solids. II. Physica Scripta, 1988, 38, 194-198.	2.5	31
95	On theab initioevaluation of Hubbard parameters. II. The Îº-(BEDT-TTF)2Cu[N(CN)2]Br crystal. Journal of Chemical Physics, 1997, 106, 8051-8058.	3.0	31
96	Designing ligand-enhanced optical absorption of thiolated gold nanoclusters. Chemical Communications, 2015, 51, 7935-7938.	4.1	31
97	Structure and Bonding of Tungsten Oxide Clusters on Nanostructured Cu-O Surfaces. Journal of Physical Chemistry C, 2011, 115, 23480-23487.	3.1	30
98	Building Principles and Structural Motifs in TiO_x Ultrathin Films on a (111) Substrate. Journal of Physical Chemistry C, 2012, 116, 13302-13306.	3.1	30
99	Atomically precise Au₁₄₄(SR)₆₀ nanoclusters (R = Et, Pr) are capped by 12 distinct ligand types of 5-fold equivalence and display gigantic diastereotopic effects. Chemical Science, 2018, 9, 8796-8805.	7.4	30
100	Density Functional Calculations of Isotropic Hyperfine Coupling Constants in .beta.-Ketoenolyl Radicals. The Journal of Physical Chemistry, 1994, 98, 8648-8652.	2.9	29
101	Structures of small Au clusters on MgO(001) studied by density-functional calculations. Physical Review B, 2011, 83, .	3.2	29
102	Communication: Kinetics of chemical ordering in Ag-Au and Ag-Ni nanoalloys. Journal of Chemical Physics, 2013, 139, 111102.	3.0	29
103	Au₂₁S(SAdm)₁₅: Crystal Structure, Mass Spectrometry, Optical Spectroscopy, and First-Principles Theoretical Analysis. Journal of Physical Chemistry C, 2017, 121, 10865-10869.	3.1	29
104	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.	3.0	29
105	Two-Dimensional Iron Tungstate: A Ternary Oxide Layer With Honeycomb Geometry. Journal of Physical Chemistry C, 2016, 120, 7629-7638.	3.1	28
106	Principles of Optical Spectroscopy of Aromatic Alloy Nanomolecules: Au_{36â€“x}Ag_x(SPh-tBu)₂₄. Journal of Physical Chemistry C, 2018, 122, 4524-4531.	3.1	28
107	Si-Doped Fe Catalyst for Ammonia Synthesis at Dramatically Decreased Pressures and Temperatures. Journal of the American Chemical Society, 2020, 142, 8223-8232.	13.7	28
108	Magic silver cluster on a MgO(100) terrace with defects. Physical Review B, 2007, 76, .	3.2	27

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109	A study of bimetallic Cuâ€“Ag, Auâ€“Ag and Pdâ€“Ag clusters adsorbed on a double-vacancy-defected MgO(100) terrace. Faraday Discussions, 2008, 138, 37-47.	3.2	27
110	Interface Effects on the Magnetism of CoPt-Supported Nanostructures. Nano Letters, 2011, 11, 5542-5547.	9.1	27
111	Reaction mechanism and kinetics for ammonia synthesis on the Fe(211) reconstructed surface. Physical Chemistry Chemical Physics, 2019, 21, 11444-11454.	2.8	27
112	Concepts in theoretical heterogeneous ultrananocatalysis. Comptes Rendus Chimie, 2014, 17, 625-633.	0.5	26
113	Discovering indium as hydrogen production booster for a Cu/SiO2 catalyst in steam reforming of methanol. Applied Catalysis B: Environmental, 2021, 297, 120398.	20.2	26
114	NWChem for materials science. Computational Materials Science, 2003, 28, 209-221.	3.0	25
115	Mobility of Au on TiO_x Substrates with Different Stoichiometry and Defectivity. Journal of Physical Chemistry C, 2008, 112, 3187-3190.	3.1	25
116	Metal adsorption on oxide polar ultrathin films. Physical Chemistry Chemical Physics, 2008, 10, 1876.	2.8	24
117	Structures of AgPd nanoclusters adsorbed on MgO(100): A computational study. Surface Science, 2011, 605, 483-488.	1.9	24
118	Metamorphosis of ultrathin Ni oxide nanostructures on Ag(100). Physical Review B, 2011, 84, .	3.2	24
119	The two-dimensional cobalt oxide (9 Ã— 2) phase on Pd(100). Journal of Chemical Physics, 2011, 134, 184706.	3.0	24
120	Work Function of Oxide Ultrathin Films on the Ag(100) Surface. Journal of Chemical Theory and Computation, 2012, 8, 629-638.	5.3	24
121	Organosoluble Au₁₀₂(SPh)₄₄ Nanomolecules: Synthesis, Isolation, Compositional Assignment, Core Conversion, Optical Spectroscopy, Electrochemistry, and Theoretical Analysis. Journal of Physical Chemistry C, 2015, 119, 25077-25084.	3.1	24
122	A new timeâ€dependent densityâ€functional method for molecular plasmonics: Formalism, implementation, and the Au₁₄₄(SH)₆₀ case study. International Journal of Quantum Chemistry, 2016, 116, 1603-1611.	2.0	24
123	Oxide Materials at the Two-Dimensional Limit. Springer Series in Materials Science, 2016, , .	0.6	24
124	Kondo effect of cobalt adatoms on nanostructured Cu-O surfaces: Scanning tunneling spectroscopy experiments and first-principles calculations. Physical Review B, 2010, 81, .	3.2	23
125	Scanning tunneling microscopy imaging of NiO(100)(1Ã—1) islands embedded in Ag(100). Surface Science, 2012, 606, 803-807.	1.9	23
126	Catalytic activity of Pt₃₈ in the oxygen reduction reaction from first-principles simulations. Catalysis Science and Technology, 2016, 6, 6901-6909.	4.1	23

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127	Laser-Beam-Patterned Topological Insulating States on Thin Semiconducting <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>MoS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn> Physical Review Letters, 2019, 123, 146803.	7.8	23
128	Reaction Mechanisms, Kinetics, and Improved Catalysts for Ammonia Synthesis from Hierarchical High Throughput Catalyst Design. Accounts of Chemical Research, 2022, 55, 1124-1134.	15.6	23
129	The dimer model for Î²-phase organic superconductors. Europhysics Letters, 1998, 42, 467-472.	2.0	22
130	Rotational Invariance and Double Frustration in the Structures of Gold Clusters Growing around the Fs-Defected MgO (100) Surface. Journal of Physical Chemistry B, 2006, 110, 21021-21027.	2.6	22
131	Diffusion of adatoms and small clusters on magnesium oxide surfaces. Journal of Physics Condensed Matter, 2009, 21, 264001.	1.8	22
132	Core-Size Conversion of Au₃₈(SCH₂CH₂Ph)₂₄ to Au₃₀(Sâ€“tBu)₁₈ Nanomolecules. Journal of Physical Chemistry C, 2017, 121, 14929-14935.	3.1	22
133	Edge Defects Promoted Oxidation of Monolayer WS₂ Synthesized on Epitaxial Graphene. Journal of Physical Chemistry C, 2020, 124, 9035-9044.	3.1	22
134	Ordered Arrays of Size-Selected Oxide Nanoparticles. Physical Review Letters, 2012, 108, 195507.	7.8	21
135	Kinetics of chemical ordering in a Ag-Pt nanoalloy particle via first-principles simulations. Journal of Chemical Physics, 2012, 137, 194302.	3.0	21
136	Nanoscale Domain Structure and Defects in a 2-D WO₃ Layer on Pd(100). Journal of Physical Chemistry C, 2016, 120, 28682-28693.	3.1	21
137	Ligand-Enhanced Optical Response of Gold Nanomolecules and Its Fragment Projection Analysis: The Case of Au₃₀(SR)₁₈. Journal of Physical Chemistry C, 2017, 121, 10832-10842.	3.1	21
138	Chirality in bare and ligand-protected metal nanoclusters. Advances in Physics: X, 2018, 3, 1509727.	4.1	21
139	Hydrogen evolution reaction (HER) on Au@Ag ultrananoclusters as electro-catalysts. Nanoscale, 2018, 10, 17730-17737.	5.6	21
140	Probing the atomic structure of metallic nanoclusters with the tip of a scanning tunneling microscope. Nanoscale, 2014, 6, 2170-2176.	5.6	20
141	Optimizing the oxygen evolution reaction for electrochemical water oxidation by tuning solvent properties. Nanoscale, 2015, 7, 4514-4521.	5.6	20
142	Highâ€Performance 2D pâ€Type Transistors Based on GaSe Layers: An Ab Initio Study. Advanced Electronic Materials, 2017, 3, 1600399.	5.1	20
143	A mixed basis set of plane waves and Hermite Gaussian functions. Analytic expressions of prototype integrals. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1987, 9, 969-977.	0.4	19
144	A simplified representation of the potential produced by Gaussian charge distributions. Journal of Computational Chemistry, 1991, 12, 36-41.	3.3	19

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145	A theoretical study of the catalytic properties of Pt/Fe nanoclusters. Computational and Theoretical Chemistry, 2002, 586, 17-27.	1.5	19
146	Directed assembly of Au and Fe nanoparticles on a TiOx/Pt(111) ultrathin template: the role of oxygen affinity. Physical Chemistry Chemical Physics, 2009, 11, 11305.	2.8	19
147	Atoms in molecules. I. A charge conservation rule for taking into account the â€˜â€˜orthogonality holeâ€™â€™. Journal of Chemical Physics, 1984, 80, 2654-2659.	3.0	18
148	Derivation of an empirical potential for gold with angular corrections. Physical Review B, 2008, 77, .	3.2	18
149	Dependence of self-diffusion coefficient, surface energy, on size, temperature, and Debye temperature on size for aluminum nanoclusters. Fluid Phase Equilibria, 2012, 335, 26-31.	2.5	18
150	Nanostripe Pattern of NaCl Layers on Cu(110). Physical Review Letters, 2013, 110, 216101.	7.8	18
151	Optical Properties of Pt and Agâ€“Pt Nanoclusters from TDDFT Calculations: Plasmon Suppression by Pt Poisoning. Journal of Physical Chemistry C, 2014, 118, 28101-28108.	3.1	18
152	Intense fluorescence of Au20. Journal of Chemical Physics, 2017, 147, 074301.	3.0	18
153	Mechanism of Protonation of [Pt3(Î¼-PBut2)3(H)(CO)2], Yielding the Hydride-Bridged [Pt3(Î¼-PBut2)2(Î¼-H)(PBut2H)(CO)2]OTf (Tf = CF3SO2), and the Spectroscopic and Theoretical Characterization of a Kinetic Intermediate. Inorganic Chemistry, 2001, 40, 3055-3060.	4.0	17
154	Au nanoparticles on a templating TiOx/Pt(111) ultrathin polar film: a photoemission and photoelectron diffraction study. Physical Chemistry Chemical Physics, 2009, 11, 2177.	2.8	17
155	Comment on â€œ(Auâ€“Ag)₁₄₄(SR)₆₀alloy nanomoleculesâ€•by C. Kumara and A. Dass, Nanoscale, 2011,3, 3064. Nanoscale, 2015, 7, 8166-8167.	5.6	17
156	Lattice Strain Defects in a Ceria Nanolayer. Journal of Physical Chemistry Letters, 2016, 7, 1303-1309.	4.6	17
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