Roy L. Johnston

List of Publications by Year in Descending Order

264 papers	12,534 citations	51 h-index	102 g-index
279 ext. papers	13,483 ext. citations	4.6 avg, IF	6.7 L-index

#	Paper	IF	Citations
264	Global minima and structural properties of Au Fe nanoalloys from a Mexican Enhanced Genetic Algorithm-based Density Functional Theory. *Chemical Physics Letters*, **2021**, 776, 138675	2.5	
263	Leveraging Hierarchical Self-Assembly Pathways for Realizing Colloidal Photonic Crystals. *ACS Nano* , **2020**, 14, 5348-5359	16.7	20
262	Effects of Hydration on the Conformational Behavior of Flexible Molecules with Two Charge Centers. *Journal of Physical Chemistry A*, **2020**, 124, 5323-5330	2.8	1
261	Structural and magnetic properties of Co-Pt clusters: A spin-polarized density functional study. *Journal of Magnetism and Magnetic Materials*, **2020**, 503, 166651	2.8	3
260	DFT-Based Global Optimization of Sub-nanometer NiPd Clusters. *Journal of Physical Chemistry C*, **2019**, 123, 26583-26596	3.8	10
259	Can a Single Valence Electron Alter the Electrocatalytic Activity and Selectivity for CO2 Reduction on the Subnanometer Scale?. *Journal of Physical Chemistry C*, **2019**, 123, 14591-14609	3.8	6
258	Tuning electronic and composition effects in ruthenium-copper alloy nanoparticles anchored on carbon nanofibers for rechargeable Li-CO2 batteries. *Chemical Engineering Journal*, **2019**, 375, 121978	14.7	26
257	Gold doping of tin clusters: exo- vs. endohedral complexes. *Nanoscale*, **2019**, 11, 12878-12888	7.7	5
256	In situ high-potential-driven surface restructuring of ternary AgPd-Pt aerogels with record-high performance improvement for formate oxidation electrocatalysis. *Nanoscale*, **2019**, 11, 14174-14185	7.7	45
255	Physico-Chemical Insights into Gas-Phase and Oxide-Supported Sub-Nanometre AuCu Clusters. *Zeitschrift Fur Physikalische Chemie*, **2019**, 233, 813-843	3.1	6
254	GIGA: a versatile genetic algorithm for free and supported clusters and nanoparticles in the presence of ligands. *Nanoscale*, **2019**, 11, 9042-9052	7.7	20
253	Altering CO binding on gold cluster cations by Pd-doping. *Nanoscale*, **2019**, 11, 16130-16141	7.7	14
252	Application of a parallel genetic algorithm to the global optimization of medium-sized AuPd sub-nanometre clusters. *European Physical Journal B*, **2018**, 91, 1	1.2	10
251	Gold-Copper Aerogels with Intriguing Surface Electronic Modulation as Highly Active and Stable Electrocatalysts for Oxygen Reduction and Borohydride Oxidation. *ChemSusChem*, **2018**, 11, 1354-1364	8.3	20
250	Modelling free and oxide-supported nanoalloy catalysts: comparison of bulk-immiscible Pd-Ir and Au-Rh systems and influence of a TiO support. *Faraday Discussions*, **2018**, 208, 53-66	3.6	14
249	A theoretical study on the geometry and spectroscopic properties of ground-state and local minima isomers of (CuS)n=2-6 clusters. *Physica E: Low-Dimensional Systems and Nanostructures*, **2018**, 97, 1-7	3	9
248	Pentameric PdAu and PdPt nanoparticles on the MgO(1 0 0) surface and their CO and O2 adsorption properties. *European Physical Journal B*, **2018**, 91, 1	1.2	5

247	Theoretical investigation of the structures of unsupported 38-atom CuPt clusters. *European Physical Journal B*, **2018**, 91, 1	1.2	7
246	Anionic cobalt-platinum-ethynyl ($CoPt_2C_2H$) metal-organic subnanoparticles: a DFT modeling study. *European Physical Journal B*, **2018**, 91, 1	1.2	1
245	Theory as a driving force to understand reactions on nanoparticles: general discussion. *Faraday Discussions*, **2018**, 208, 147-185	3.6	1
244	The challenges of characterising nanoparticulate catalysts: general discussion. *Faraday Discussions*, **2018**, 208, 339-394	3.6	4
243	Chemical bonding in initial building blocks of semiconductors: Geometrical structures and optical absorption spectra of isolated and Cd species. *Journal of Chemical Physics*, **2018**, 149, 244308	3.9	6
242	Isomers and energy landscapes of micro-hydrated sulfite and chlorate clusters. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2018**, 376,	3	3
241	The DFT-genetic algorithm approach for global optimization of subnanometer bimetallic clusters. *Frontiers of Nanoscience*, **2018**, 12, 145-169	0.7	6
240	First principles global optimization of metal clusters and nanoalloys. *Advances in Physics: X*, **2018**, 3, S100009	5.6	15
239	AgSn intermetallics as highly selective and active oxygen reduction electrocatalysts in membraneless alkaline fuel cells. *Journal of Power Sources*, **2018**, 404, 106-117	8.9	17
238	Effect of palladium doping on the stability and fragmentation patterns of cationic gold clusters. *Physical Review A*, **2018**, 97,	2.6	21
237	DFT Global Optimization of Gas-Phase Subnanometer Ru_nPt Clusters. *Journal of Physical Chemistry C*, **2017**, 121, 10773-10780	3.8	30
236	Activity Trends of Binary Silver Alloy Nanocatalysts for Oxygen Reduction Reaction in Alkaline Media. *Small*, **2017**, 13, 1603387	11	38
235	One-Pot Synthesis of Dealloyed AuNi Nanodendrite as a Bifunctional Electrocatalyst for Oxygen Reduction and Borohydride Oxidation Reaction. *Advanced Functional Materials*, **2017**, 27, 1700260	15.6	33
234	A DFT study of molecular adsorption on titania-supported AuRh nanoalloys. *Computational and Theoretical Chemistry*, **2017**, 1107, 142-151	2	14
233	Engineering Bimetallic Ag-Cu Nanoalloys for Highly Efficient Oxygen Reduction Catalysts: A Guideline for Designing Ag-Based Electrocatalysts with Activity Comparable to Pt/C-20. *Small*, **2017**, 13, 1603876	11	21
232	Bifunctional Electrocatalysts for Oxygen Reduction and Borohydride Oxidation Reactions Using AgSn Nanointermetallic for the Ensemble Effect. *ACS Applied Materials & Interfaces*, **2017**, 9, 35701-35711	9.5	18
231	DFT study of the structure, chemical ordering and molecular adsorption of Pd-Ir nanoalloys. *Physical Chemistry Chemical Physics*, **2017**, 19, 27090-27098	3.6	12
230	Study of the stability of small AuRh clusters found by a Genetic Algorithm methodology. *Computational and Theoretical Chemistry*, **2017**, 1119, 51-58	2	13

229	Adsorption of Acetonitrile, Benzene, and Benzonitrile on Pt(111): Single Crystal Adsorption Calorimetry and Density Functional Theory. *Journal of Physical Chemistry C*, **2017**, 121, 21354-21363	3.8	14
228	Reduced Graphene Oxide decorated with Manganese Cobalt Oxide as Multifunctional Material for Mechanically Rechargeable and Hybrid Zinc□Air Batteries. *Particle and Particle Systems Characterization*, **2017**, 34, 1700097	3.1	36
227	Size effect on the adsorption and dissociation of CO2 on Co nanoclusters. *Applied Surface Science*, **2017**, 396, 539-546	6.7	19
226	Investigation of the Structures and Energy Landscapes of Thiocyanate-Water Clusters. *Inorganics*, **2017**, 5, 20	2.9	3
225	Global Optimisation Strategies for Nanoalloys. *Challenges and Advances in Computational Chemistry and Physics*, **2017**, 1-52	0.7	
224	DFT global optimisation of gas-phase and MgO-supported sub-nanometre AuPd clusters. *Physical Chemistry Chemical Physics*, **2016**, 18, 26133-26143	3.6	28
223	A comparative study of AumRhn (4 □m + n □6) clusters in the gas phase versus those deposited on (100) MgO. *Physical Chemistry Chemical Physics*, **2016**, 18, 22122-8	3.6	10
222	Highly active and stable AuNi dendrites as an electrocatalyst for the oxygen reduction reaction in alkaline media. *Journal of Materials Chemistry A*, **2016**, 4, 17828-17837	13	30
221	A silver□copper metallic glass electrocatalyst with high activity and stability comparable to Pt/C for zinc□air batteries. *Journal of Materials Chemistry A*, **2016**, 4, 3527-3537	13	42
220	Charge and Compositional Effects on the 2D□3D Transition in Octameric AgAu Clusters. *Zeitschrift Fur Physikalische Chemie*, **2016**, 230, 955-975	3.1	7
219	Global optimization of small bimetallic Pd-Co binary nanoalloy clusters: a genetic algorithm approach at the DFT level. *Physical Chemistry Chemical Physics*, **2016**, 18, 6676-82	3.6	32
218	Application of a Parallel Genetic Algorithm to the Global Optimization of Gas-Phase and Supported Gold□Iridium Sub-Nanoalloys. *Journal of Physical Chemistry C*, **2016**, 120, 3759-3765	3.8	24
217	Pt-free silver nanoalloy electrocatalysts for oxygen reduction reaction in alkaline media. *Catalysis Science and Technology*, **2016**, 6, 3317-3340	5.5	75
216	A DFT study of molecular adsorption on AuRh nanoalloys. *Catalysis Science and Technology*, **2016**, 6, 6916-6931	5.5	20
215	Optical Absorption of Small Palladium-Doped Gold Clusters. *Particle and Particle Systems Characterization*, **2016**, 33, 364-372	3.1	22
214	Optical Absorption: Optical Absorption of Small Palladium-Doped Gold Clusters (Part. Part. Syst. Charact. 7/2016). *Particle and Particle Systems Characterization*, **2016**, 33, 363-363	3.1	
213	Understanding and controlling the structure and segregation behaviour of AuRh nanocatalysts. *Scientific Reports*, **2016**, 6, 35226	4.9	37
212	Isomers and Energy Landscapes of Perchlorate-Water Clusters and a Comparison to Pure Water and Sulfate-Water Clusters. *Journal of Physical Chemistry A*, **2016**, 120, 4008-15	2.8	18

211	Structural evolution and metallicity of lead clusters. *Nanoscale*, **2016**, 8, 11153-60	7.7	14
210	A Threshold-Minimization Scheme for Exploring the Energy Landscape of Biomolecules: Application to a Cyclic Peptide and a Disaccharide. *Journal of Chemical Theory and Computation*, **2016**, 12, 2471-9	6.4	5
209	O2 Dissociation on Core□Shell Particles for 3d, 4d, and 5d Transition Metals. *Journal of Physical Chemistry C*, **2015**, 119, 11031-11041	3.8	35
208	Silver-Copper Nanoalloy Catalyst Layer for Bifunctional Air Electrodes in Alkaline Media. *ACS Applied Materials & Interfaces*, **2015**, 7, 17782-91	9.5	60
207	The Birmingham parallel genetic algorithm and its application to the direct DFT global optimisation of Ir(N) (N = 10-20) clusters. *Nanoscale*, **2015**, 7, 14032-8	7.7	56
206	Optical absorption spectra and structures of Ag +6 and Ag +8. *European Physical Journal D*, **2015**, 69, 1	1.3	15
205	Computational study of the adsorption of benzene and hydrogen on palladium□iridium nanoalloys. *Journal of Organometallic Chemistry*, **2015**, 792, 190-193	2.3	7
204	Structures and Energy Landscapes of Hydrated Sulfate Clusters. *Journal of Chemical Theory and Computation*, **2015**, 11, 2377-84	6.4	27
203	Energy landscape exploration of sub-nanometre copper-silver clusters. *ChemPhysChem*, **2015**, 16, 1461-9	3.2	18
202	Theoretical study of the structures and chemical ordering of cobalt-palladium nanoclusters. *Physical Chemistry Chemical Physics*, **2015**, 17, 28311-21	3.6	32
201	The Nature of Bonding between Argon and Mixed Gold-Silver Trimers. *Angewandte Chemie - International Edition*, **2015**, 54, 10675-80	16.4	54
200	The Effect of Dispersion Correction on the Adsorption of CO on Metallic Nanoparticles. *Journal of Physical Chemistry A*, **2015**, 119, 9703-9	2.8	48
199	Pool-BCGA: a parallelised generation-free genetic algorithm for the ab initio global optimisation of nanoalloy clusters. *Physical Chemistry Chemical Physics*, **2015**, 17, 2104-12	3.6	72
198	Charge-induced dipole vs. relativistically enhanced covalent interactions in Ar-tagged Au-Ag tetramers and pentamers. *Journal of Chemical Physics*, **2015**, 143, 024310	3.9	31
197	Chiral effects on helicity studied via the energy landscape of short (D, L)-alanine peptides. *Journal of Chemical Physics*, **2015**, 143, 165103	3.9	7
196	Zum Charakter der chemischen Bindung von Argonatomen mit gemischten Gold/Silber-Trimeren. *Angewandte Chemie*, **2015**, 127, 10822-10827	3.6	6
195	Global optimization of 8-10 atom palladium-iridium nanoalloys at the DFT level. *Journal of Physical Chemistry A*, **2014**, 118, 208-14	2.8	24
194	Pd(n)Ag(4-n) and Pd(n)Pt(4-n) clusters on MgO (100): a density functional surface genetic algorithm investigation. *Nanoscale*, **2014**, 6, 11777-88	7.7	31

193	Visualizing energy landscapes with metric disconnectivity graphs. *Journal of Computational Chemistry*, **2014**, 35, 1481-90	3.5	19
192	Support and Oxidation Effects on Subnanometer Palladium Nanoparticles. *Journal of Physical Chemistry C*, **2014**, 118, 3581-3589	3.8	19
191	Modeling nanoscale inhomogeneities for quantitative HAADF STEM imaging. *Physical Review Letters*, **2014**, 113, 075501	7.4	18
190	A theoretical study of the structures and optical spectra of helical copper-silver clusters. *Physical Chemistry Chemical Physics*, **2014**, 16, 21039-48	3.6	12
189	DFT studies of oxygen dissociation on the 116-atom platinum truncated octahedron particle. *Physical Chemistry Chemical Physics*, **2014**, 16, 26539-45	3.6	20
188	Energy Landscapes and Global Optimization of Self-Assembling Cyclic Peptides. *Journal of Chemical Theory and Computation*, **2014**, 10, 1810-6	6.4	14
187	Structure and solid solution properties of Cu-Ag nanoalloys. *Journal of Physics Condensed Matter*, **2014**, 26, 275301	1.8	32
186	Optical and electronic properties of mixed Ag-Au tetramer cations. *Journal of Chemical Physics*, **2014**, 140, 054312	3.9	39
185	Comparative modelling of chemical ordering in palladium-iridium nanoalloys. *Journal of Chemical Physics*, **2014**, 141, 224307	3.9	21
184	Interfacial Structures and Bonding in Metal-Coated Gold Nanorods. *Structure and Bonding*, **2014**, 67-90	0.9	5
183	Communication: Global minimum search of Ag with molecular beam optical spectroscopy. *Journal of Chemical Physics*, **2014**, 141, 181104	3.9	13
182	Influence of spin-orbit effects on structures and dielectric properties of neutral lead clusters. *Journal of Chemical Physics*, **2014**, 140, 164313	3.9	12
181	A DFT study of oxygen dissociation on platinum based nanoparticles. *Nanoscale*, **2014**, 6, 1153-1165	7.7	56
180	Effect of CO and H adsorption on the compositional structure of binary nanoalloys via DFT modeling. *European Physical Journal D*, **2013**, 67, 1	1.3	13
179	Theoretical Study of the Structures and Chemical Ordering of Palladium Gold Nanoalloys Supported on MgO(100). *Journal of Physical Chemistry C*, **2013**, 117, 293-301	3.8	27
178	Improving the Adsorption of Au Atoms and Nanoparticles on Graphite via Li Intercalation. *Journal of Physical Chemistry C*, **2013**, 117, 22683-22695	3.8	4
177	Global minimum Pt(13)M(20) (M = Ag, Au, Cu, Pd) dodecahedral core-shell clusters. *Journal of Physical Chemistry A*, **2013**, 117, 14261-6	2.8	26
176	Structures of small Ti- and V-doped Pt clusters: A GA-DFT study. *Computational and Theoretical Chemistry*, **2013**, 1021, 91-100	2	19

175	A density functional global optimisation study of neutral 8-atom Cu-Ag and Cu-Au clusters. *European Physical Journal D*, **2013**, 67, 1	1.3	37
174	Evaluation of photodissociation spectroscopy as a structure elucidation tool for isolated clusters: a case study of Ag4(+) and Au4(+). *Physical Chemistry Chemical Physics*, **2013**, 15, 19715-23	3.6	34
173	Determination of the energy landscape of Pd12Pt1 using a combined genetic algorithm and threshold energy method. *RSC Advances*, **2013**, 3, 11571	3.7	11
172	Direct atomic imaging and density functional theory study of the Au24Pd1 cluster catalyst. *Nanoscale*, **2013**, 5, 9620-5	7.7	32
171	Symmetrisation schemes for global optimisation of atomic clusters. *Physical Chemistry Chemical Physics*, **2013**, 15, 3965-76	3.6	51
170	Protein structure optimization with a "Lamarckian" ant colony algorithm. *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, **2013**, 10, 1548-52	3	3
169	DFT study of the structures and energetics of 98-atom AuPd clusters. *Nanoscale*, **2013**, 5, 646-52	7.7	52
168	Faceting preferences for Au(N) and Pd(N) nanoclusters with high-symmetry motifs. *Physical Chemistry Chemical Physics*, **2013**, 15, 8392-400	3.6	9
167	Modelling the metal-on-top effect for Pd clusters on the MgO{100} substrate. *Journal of Chemical Physics*, **2013**, 138, 224703	3.9	10
166	Global optimization of clusters using electronic structure methods. *International Journal of Quantum Chemistry*, **2013**, 113, 2091-2109	2.1	155
165	Size-dependent subnanometer Pd cluster (Pd4, Pd6, and Pd17) water oxidation electrocatalysis. *ACS Nano*, **2013**, 7, 5808-17	16.7	125
164	An atomistic view of the interfacial structures of AuRh and AuPd nanorods. *Nanoscale*, **2013**, 5, 7452-7	7.7	42
163	A selective blocking method to control the overgrowth of Pt on Au nanorods. *Journal of the American Chemical Society*, **2013**, 135, 6554-61	16.4	72
162	Computational and experimental investigations into the conformations of cyclic tetra-Ala peptides. *Journal of Physical Chemistry B*, **2013**, 117, 8122-34	3.4	17
161	Exploring the Energy Landscapes of Cyclic Tetrapeptides with Discrete Path Sampling. *Journal of Chemical Theory and Computation*, **2013**, 9, 650-657	6.4	32
160	Low-loss optical magnetic metamaterials on Ag/Au bimetallic fishnets. *Journal of Magnetism and Magnetic Materials*, **2012**, 324, 2625-2630	2.8	6
159	Development and optimization of a novel genetic algorithm for identifying nanoclusters from scanning transmission electron microscopy images. *Journal of Computational Chemistry*, **2012**, 33, 391-400	3.5	15
158	Electronic Properties of Pt/Ti Nanoalloys and the Effect on Reactivity for Use in PEMFCs. *Journal of Physical Chemistry C*, **2012**, 116, 15241-15250	3.8	19

157	Overgrowth of Rhodium on Gold Nanorods. *Journal of Physical Chemistry C*, **2012**, 116, 10312-10317	3.8	28
156	Metal Nanoparticles and Nanoalloys. *Frontiers of Nanoscience*, **2012**, 3, 1-42	0.7	43
155	Theoretical studies of Pt-Ti nanoparticles for potential use as PEMFC electrocatalysts. *Physical Chemistry Chemical Physics*, **2012**, 14, 3134-9	3.6	31
154	Interdependence of structure and chemical order in high symmetry (PdAu)N nanoclusters. *RSC Advances*, **2012**, 2, 5863	3.7	16
153	Predicting the Optical Properties of Core–Shell and Janus Segregated Au–M Nanoparticles (M = Ag, Pd). *Journal of Physical Chemistry C*, **2012**, 116, 23616-23628	3.8	30
152	Tetrahelix conformations and transformation pathways in Pt1Pd12 clusters. *Journal of Physical Chemistry A*, **2012**, 116, 5235-9	2.8	14
151	Dopant-induced 2D-3D transition in small Au-containing clusters: DFT-global optimisation of 8-atom Au-Ag nanoalloys. *Nanoscale*, **2012**, 4, 1109-15	7.7	87
150	Nine-Atom Tin-Bismuth Clusters: Mimicking Excess Electrons by Element Substitution. *ChemPlusChem*, **2012**, 77, 532-535	2.8	15
149	Bismuth-doped tin clusters: experimental and theoretical studies of neutral Zintl analogues. *Journal of Physical Chemistry A*, **2012**, 116, 7756-64	2.8	28
148	Configuration of microbially synthesized Pd-Au nanoparticles studied by STEM-based techniques. *Nanotechnology*, **2012**, 23, 055701	3.4	10
147	Note: gas phase structures of bare Si8 and Si11 clusters from molecular beam electric deflection experiments. *Journal of Chemical Physics*, **2012**, 136, 186101	3.9	21
146	The Effect of Nonnative Interactions on the Energy Landscapes of Frustrated Model Proteins. *Journal of Atomic, Molecular, and Optical Physics*, **2012**, 2012, 1-9		3
145	Energy landscape and global optimization for a frustrated model protein. *Journal of Physical Chemistry B*, **2011**, 115, 11525-9	3.4	29
144	Surface reconstruction precursor to melting in Au309 clusters. *AIP Advances*, **2011**, 1, 032105	1.5	5
143	Collective plasmon modes in a compositionally asymmetric nanoparticle dimer. *AIP Advances*, **2011**, 1, 032134	1.5	44
142	TEM characterization of chemically synthesized copper–gold nanoparticles. *Journal of Nanoparticle Research*, **2011**, 13, 4229-4237	2.3	13
141	Study of 40-atom Pt–Au clusters using a combined empirical potential-density functional approach. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, **2011**, 467, 2004-2019	2.4	34
140	Truncated-octahedral copper-gold nanoparticles. *Journal of Physics: Conference Series*, **2010**, 241, 012086	0.3	2

139	Theoretical and Experimental Studies of the Optical Properties of Conjoined Gold–Palladium Nanospheres. *Journal of Physical Chemistry C*, **2010**, 114, 21247-21251	3.8	13
138	Structures and Chemical Ordering of Small Cu–Ag Clusters. *Journal of Physical Chemistry C*, **2010**, 114, 13255-13266	3.8	81
137	The Effect of CO and H Chemisorption on the Chemical Ordering of Bimetallic Clusters. *Journal of Physical Chemistry C*, **2010**, 114, 19678-19686	3.8	41
136	Investigation of the structures and chemical ordering of small Pd-Au clusters as a function of composition and potential parameterisation. *Physical Chemistry Chemical Physics*, **2010**, 12, 8607-19	3.6	53
135	Energetic and Structural Analysis of 102-Atom Pd–Pt Nanoparticles: A Composition-Dependent Study. *Journal of Computational and Theoretical Nanoscience*, **2010**, 7, 199-204	0.3	9
134	Structures and Stabilities of Platinum–Gold Nanoclusters. *Journal of Computational and Theoretical Nanoscience*, **2009**, 6, 857-866	0.3	41
133	Plasmonic Properties of Silver Nanoparticles on Two Substrates. *Plasmonics*, **2009**, 4, 147-152	2.4	29
132	Chemisorption of CO and H on Pd, Pt and Au nanoclusters: a DFT approach. *European Physical Journal D*, **2009**, 52, 131-134	1.3	35
131	Analysis of the X-ray absorption fine structure near the TiL 2, 3 edge in free titanium nanoclusters. *Journal of Surface Investigation*, **2009**, 3, 38-40	0.5	0
130	Small Copper Clusters in Ar Shells: A Study of Local Structure. *Journal of Physical Chemistry C*, **2009**, 113, 9086-9091	3.8	18
129	Structural Insights into 19-Atom Pd/Pt Nanoparticles: A Computational Perspective. *Journal of Physical Chemistry C*, **2009**, 113, 15904-15908	3.8	20
128	Theoretical Studies of Palladium–Gold Nanoclusters: Pd–Au Clusters with up to 50 Atoms. *Journal of Physical Chemistry C*, **2009**, 113, 9141-9152	3.8	144
127	Theoretical study of Cu(38-n)Au(n) clusters using a combined empirical potential-density functional approach. *Physical Chemistry Chemical Physics*, **2009**, 11, 10340-9	3.6	35
126	Three-dimensional atomic-scale structure of size-selected gold nanoclusters. *Nature*, **2008**, 451, 46-8	50.4	371
125	Nanoalloys: from theory to application. Preface. *Faraday Discussions*, **2008**, 138, 9-10	3.6	15
124	Structures and optical properties of 4-5 nm bimetallic AgAu nanoparticles. *Faraday Discussions*, **2008**, 138, 363-73; discussion 421-34	3.6	93
123	Energetic, electronic, and thermal effects on structural properties of Ag-Au nanoalloys. *ACS Nano*, **2008**, 2, 165-75	16.7	53
122	Structural motifs, mixing, and segregation effects in 38-atom binary clusters. *Journal of Chemical Physics*, **2008**, 128, 134517	3.9	136

121	Dependence of the structures and chemical ordering of PdPt nanoalloys on potential parameters. *Journal of Materials Chemistry*, **2008**, 18, 4154		40
120	Charge transfer driven surface segregation of gold atoms in 13-atom AuAg nanoalloys and its relevance to their structural, optical and electronic properties. *Acta Materialia*, **2008**, 56, 2374-2380	8.4	80
119	Martensitic transformations in AgAu bimetallic core-shell nanoalloys. *Applied Physics Letters*, **2008**, 92, 023112	3.4	40
118	Nanoalloys: from theory to applications of alloy clusters and nanoparticles. *Chemical Reviews*, **2008**, 108, 845-910	68.1	2867
117	Searching for the optimum structures of alloy nanoclusters. *Physical Chemistry Chemical Physics*, **2008**, 10, 640-9	3.6	170
116	Three-dimensional atomic-scale structure of size-selected nanoclusters on surfaces **2008**, 133-134		
115	Structure, Melting, and Thermal Stability of 55 Atom AgAu Nanoalloys. *Journal of Physical Chemistry C*, **2007**, 111, 9157-9165	3.8	68
114	Structures and energetics of 98 atom Pd-Pt nanoalloys: potential stability of the Leary tetrahedron for bimetallic nanoparticles. *Physical Chemistry Chemical Physics*, **2007**, 9, 5202-8	3.6	77
113	Combining Theory and Experiment to Characterize the Atomic Structures of Surface-Deposited Au309 Clusters *Journal of Physical Chemistry C*, **2007**, 111, 17846-17851	3.8	31
112	Advantages of a redefinition of variable-space in direct-space structure solution from powder x-ray diffraction data. *ChemPhysChem*, **2007**, 8, 650-3	3.2	14
111	Theoretical investigations of nanopatterning on the Au(1 1 1) surface. *Surface Science*, **2007**, 601, 4175-4179	1.8	2
110	Theoretical study of structure and segregation in 38-atom Ag-Au nanoalloys. *European Physical Journal D*, **2007**, 43, 53-56	1.3	32
109	Structure and spectral characteristics of the nanoalloy Ag3Au10. *Applied Physics Letters*, **2007**, 90, 153123	3.4	50
108	Nanofinger growth on Au(111) arising from kinetic instability. *Physical Review B*, **2007**, 75,	3.3	4
107	A Mixed Structural Motif in 34-Atom PdPt Clusters. *Journal of Physical Chemistry C*, **2007**, 111, 2936-2941	3.8	86
106	Analyzing energy landscapes for folding model proteins. *Journal of Chemical Physics*, **2006**, 124, 204714	3.9	3
105	Topographical complexity of multidimensional energy landscapes. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 18551-5	11.5	32
104	Spectroscopy of growing and evaporating water droplets: exploring the variation in equilibrium droplet size with relative humidity. *Journal of Physical Chemistry A*, **2006**, 110, 8116-25	2.8	76

103	Characterizing potential surface topographies through the distribution of saddles and minima. *Journal of Physical Chemistry A*, **2006**, 110, 11543-50	2.8	9
102	Atom ordering in cuboctahedral Ni$_{13}$Al nanoalloys. *Inorganica Chimica Acta*, **2006**, 359, 3649-3658	2.7	15
101	Global optimization of bimetallic cluster structures. I. Size-mismatched Ag-Cu, Ag-Ni, and Au-Cu systems. *Journal of Chemical Physics*, **2005**, 122, 194308	3.9	276
100	How many dimensions are required to approximate the potential energy landscape of a model protein?. *Journal of Chemical Physics*, **2005**, 122, 84714	3.9	49
99	Global optimization of bimetallic cluster structures. II. Size-matched Ag-Pd, Ag-Au, and Pd-Pt systems. *Journal of Chemical Physics*, **2005**, 122, 194309	3.9	180
98	Strategies for increasing the efficiency of a genetic algorithm for the structural optimization of nanoalloy clusters. *Journal of Computational Chemistry*, **2005**, 26, 1069-78	3.5	35
97	Developments in genetic algorithm techniques for structure solution from powder diffraction data. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2004**, 219, 838-846	1	63
96	Ammonium cyanate: a DFT study of crystal structure, rotational barriers and vibrational spectrum. *Molecular Physics*, **2004**, 102, 869-876	1.7	5
95	Development and optimisation of a novel genetic algorithm for studying model protein folding. *Theoretical Chemistry Accounts*, **2004**, 112, 163	1.9	22
94	Rationalizing the structural properties of bupivacaine base--a local anesthetic--directly from powder X-ray diffraction data. *Journal of Pharmaceutical Sciences*, **2004**, 93, 667-74	3.9	9
93	An efficient algorithm for calculating whole-profile functions in crystal structure solution from powder diffraction data. *Chemical Physics Letters*, **2004**, 390, 394-398	2.5	4
92	Fundamental Developments in Direct-Space Techniques for Structure Solution from Powder Diffraction Data. *Materials Science Forum*, **2004**, 443-444, 11-22	0.4	
91	Powder Diffraction Indexing as a Pattern Recognition Problem: A New Approach for Unit Cell Determination Based on an Artificial Neural Network. *Journal of Physical Chemistry A*, **2004**, 108, 711-716	2.8	9
90	Theoretical investigation of isomer stability in platinum–palladium nanoalloy clusters. *Journal of Materials Chemistry*, **2004**, 14, 1691-1704		79
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