Roy L. Johnston

List of Publications by Citations

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	Nanoalloys: from theory to applications of alloy clusters and nanoparticles. *Chemical Reviews*, **2008**, 108, 845-910	68.1	2867
263	Evolving better nanoparticles: Genetic algorithms for optimising cluster geometries. *Dalton Transactions*, **2003**, 4193	4.3	491
262	Three-dimensional atomic-scale structure of size-selected gold nanoclusters. *Nature*, **2008**, 451, 46-8	50.4	371
261	Theoretical study of Cu□Au nanoalloy clusters using a genetic algorithm. *Journal of Chemical Physics* , **2002**, 116, 1536-1550	3.9	306
260	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
259	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
258	The application of a genetic algorithm for solving crystal structures from powder diffraction data. *Chemical Physics Letters*, **1997**, 280, 189-195	2.5	170
257	Searching for the optimum structures of alloy nanoclusters. *Physical Chemistry Chemical Physics*, **2008**, 10, 640-9	3.6	170
256	Global optimization of clusters using electronic structure methods. *International Journal of Quantum Chemistry*, **2013**, 113, 2091-2109	2.1	155
255	The Genetic Algorithm: Foundations and Apllications in Structure Solution from Powder Diffraction Data. *Acta Crystallographica Section A: Foundations and Advances*, **1998**, 54, 632-645		150
254	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
253	Structural motifs, mixing, and segregation effects in 38-atom binary clusters. *Journal of Chemical Physics*, **2008**, 128, 134517	3.9	136
252	Size-dependent subnanometer Pd cluster (Pd4, Pd6, and Pd17) water oxidation electrocatalysis. *ACS Nano*, **2013**, 7, 5808-17	16.7	125
251	Investigation of the structures of MgO clusters using a genetic algorithm. *Physical Chemistry Chemical Physics*, **2001**, 3, 5024-5034	3.6	123
250	Superdense carbon, C8: supercubane or analog of .gamma.-silicon?. *Journal of the American Chemical Society*, **1989**, 111, 810-819	16.4	120
249	Theoretical models of cluster bonding. *Structure and Bonding*, **1987**, 29-87	0.9	119
248	A genetic algorithm for the structural optimization of Morse clusters. *Theoretical Chemistry Accounts*, **2000**, 104, 123-130	1.9	115

247	Geometries and segregation properties of platinum–palladium nanoalloy clusters. *Dalton Transactions RSC*, **2002**, 4375		112
246	Structure-Bonding Relationships in the Laves Phases. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **1992**, 616, 105-120	1.3	103
245	Relative electron donor strengths of tetrathiafulvene derivatives: effects of chemical substitutions and the molecular environment from a combined photoelectron and electrochemical study. *Journal of the American Chemical Society*, **1990**, 112, 3302-3307	16.4	97
244	Structures and optical properties of 4-5 nm bimetallic AgAu nanoparticles. *Faraday Discussions*, **2008**, 138, 363-73; discussion 421-34	3.6	93
243	Atomic and Molecular Clusters		89
242	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
241	Implementation of Lamarckian concepts in a Genetic Algorithm for structure solution from powder diffraction data. *Chemical Physics Letters*, **2000**, 321, 183-190	2.5	87
240	A Mixed Structural Motif in 34-Atom Pd–Pt Clusters. *Journal of Physical Chemistry C*, **2007**, 111, 2936-2941	3.8	86
239	Molecular orbital calculations relevant to the hypercloso vs. iso-closo controversy in metallaboranes. *Inorganic Chemistry*, **1986**, 25, 3321-3323	5.1	85
238	A theoretical study of atom ordering in copper–gold nanoalloy clusters. *Journal of Materials Chemistry*, **2002**, 12, 2913-2922		83
237	Structures and Chemical Ordering of Small Cu–Ag Clusters. *Journal of Physical Chemistry C*, **2010**, 114, 13255-13266	3.8	81
236	Charge transfer driven surface segregation of gold atoms in 13-atom Au–Ag nanoalloys and its relevance to their structural, optical and electronic properties. *Acta Materialia*, **2008**, 56, 2374-2380	8.4	80
235	Theoretical investigation of isomer stability in platinum–palladium nanoalloy clusters. *Journal of Materials Chemistry*, **2004**, 14, 1691-1704		79
234	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
233	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
232	Pt-free silver nanoalloy electrocatalysts for oxygen reduction reaction in alkaline media. *Catalysis Science and Technology*, **2016**, 6, 3317-3340	5.5	75
231	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
230	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

229	The development of metallic behaviour in clusters. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **1998**, 356, 211-230	3	71
228	Structure, Melting, and Thermal Stability of 55 Atom AgAu Nanoalloys. *Journal of Physical Chemistry C*, **2007**, 111, 9157-9165	3.8	68
227	Modelling aluminium clusters with an empirical many-body potential. *Chemical Physics*, **1998**, 236, 107-121	2.3	64
226	Developments in genetic algorithm techniques for structure solution from powder diffraction data. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2004**, 219, 838-846	1	63
225	Modeling calcium and strontium clusters with many-body potentials. *Journal of Chemical Physics*, **1997**, 107, 4674-4687	3.9	62
224	Silver-Copper Nanoalloy Catalyst Layer for Bifunctional Air Electrodes in Alkaline Media. *ACS Applied Materials & Interfaces*, **2015**, 7, 17782-91	9.5	60
223	Structures, stabilities and ordering in Ni-Al nanoalloy clusters. *European Physical Journal D*, **2003**, 25, 41-55	1.3	57
222	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
221	A DFT study of oxygen dissociation on platinum based nanoparticles. *Nanoscale*, **2014**, 6, 1153-1165	7.7	56
220	Development of a multipopulation parallel genetic algorithm for structure solution from powder diffraction data. *Journal of Computational Chemistry*, **2003**, 24, 1766-74	3.5	55
219	The Nature of Bonding between Argon and Mixed Gold-Silver Trimers. *Angewandte Chemie - International Edition*, **2015**, 54, 10675-80	16.4	54
218	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
217	Energetic, electronic, and thermal effects on structural properties of Ag-Au nanoalloys. *ACS Nano*, **2008**, 2, 165-75	16.7	53
216	Structure determination of a steroid directly from powder diffraction data *Chemical Communications*, **1999**, 1677-1678	5.8	53
215	DFT study of the structures and energetics of 98-atom AuPd clusters. *Nanoscale*, **2013**, 5, 646-52	7.7	52
214	Structure Determination of an Oligopeptide Directly from Powder Diffraction Data. *Angewandte Chemie - International Edition*, **2000**, 39, 4488-4491	16.4	52
213	Symmetrisation schemes for global optimisation of atomic clusters. *Physical Chemistry Chemical Physics*, **2013**, 15, 3965-76	3.6	51
212	Determination of main structural compositions of nanoalloy clusters of CuxAuy (x + y 30) using a genetic algorithm approach. *International Journal of Quantum Chemistry*, **2003**, 95, 112-125	2.1	51

211	Evolving Opportunities in Structure Solution from Powder Diffraction Data-Crystal Structure Determination of a Molecular System with Twelve Variable Torsion Angles. *Angewandte Chemie - International Edition*, **1999**, 38, 831-835	16.4	51
210	Structure and spectral characteristics of the nanoalloy Ag3Au10. *Applied Physics Letters*, **2007**, 90, 153123	3.4	50
209	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
208	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
207	Empirical Potentials for Modeling Solids, Surfaces, and Clusters. *Journal of Solid State Chemistry*, **1999**, 145, 517-540	3.3	47
206	C-HtriplebondO hydrogen bond mediated chain reversal in a peptide containing a gamma-amino acid residue, determined directly from powder X-ray diffraction data. *Angewandte Chemie - International Edition*, **2002**, 41, 494-6	16.4	46
205	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
204	Collective plasmon modes in a compositionally asymmetric nanoparticle dimer. *AIP Advances*, **2011**, 1, 032134	1.5	44
203	Definition of a γguiding functionNn global optimization: a hybrid approach combining energy and R-factor in structure solution from powder diffraction data. *Chemical Physics Letters*, **2000**, 317, 296-303	2.5	44
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199	An atomistic view of the interfacial structures of AuRh and AuPd nanorods. *Nanoscale*, **2013**, 5, 7452-7	7.7	42
198	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
197	Structures and Stabilities of Platinum□Gold Nanoclusters. *Journal of Computational and Theoretical Nanoscience*, **2009**, 6, 857-866	0.3	41
196	Dependence of the structures and chemical ordering of Pd□Pt nanoalloys on potential parameters. *Journal of Materials Chemistry*, **2008**, 18, 4154		40
195	Martensitic transformations in Ag□Au bimetallic core-shell nanoalloys. *Applied Physics Letters*, **2008**, 92, 023112	3.4	40
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192	Investigation of geometric shell aluminum clusters using the Gupta many-body potential. *Journal of Chemical Physics*, **2000**, 112, 4773-4778	3.9	39
191	Cluster structures and stabilities from solid-state potentials. Application to silicon clusters. *Journal of the Chemical Society, Faraday Transactions*, **1992**, 88, 1229		39
190	Activity Trends of Binary Silver Alloy Nanocatalysts for Oxygen Reduction Reaction in Alkaline Media. *Small*, **2017**, 13, 1603387	11	38
189	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
188	New Light on an Old Story:´ The Solid-State Transformation of Ammonium Cyanate into Urea. *Journal of the American Chemical Society*, **1998**, 120, 13274-13275	16.4	37
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186	Understanding and controlling the structure and segregation behaviour of AuRh nanocatalysts. *Scientific Reports*, **2016**, 6, 35226	4.9	37
185	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
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183	O2 Dissociation on [email´protected] Core–Shell Particles for 3d, 4d, and 5d Transition Metals. *Journal of Physical Chemistry C*, **2015**, 119, 11031-11041	3.8	35
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180	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
179	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
178	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
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172	Exploring the Energy Landscapes of Cyclic Tetrapeptides with Discrete Path Sampling. *Journal of Chemical Theory and Computation*, **2013**, 9, 650-657	6.4	32
171	Theoretical study of structure and segregation in 38-atom Ag-Au nanoalloys. *European Physical Journal D*, **2007**, 43, 53-56	1.3	32
170	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
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165	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
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156	Bismuth-doped tin clusters: experimental and theoretical studies of neutral Zintl analogues. *Journal of Physical Chemistry A*, **2012**, 116, 7756-64	2.8	28
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136	Comparative modelling of chemical ordering in palladium-iridium nanoalloys. *Journal of Chemical Physics*, **2014**, 141, 224307	3.9	21
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132	Leveraging Hierarchical Self-Assembly Pathways for Realizing Colloidal Photonic Crystals. *ACS Nano*, **2020**, 14, 5348-5359	16.7	20
131	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
130	DFT studies of oxygen dissociation on the 116-atom platinum truncated octahedron particle. *Physical Chemistry Chemical Physics*, **2014**, 16, 26539-45	3.6	20
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122	Structures of small Ti- and V-doped Pt clusters: A GA-DFT study. *Computational and Theoretical Chemistry*, **2013**, 1021, 91-100	2	19

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102	Optical absorption spectra and structures of Ag +6 and Ag +8. *European Physical Journal D*, **2015**, 69, 1	1.3	15
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100	Nine-Atom Tin-Bismuth Clusters: Mimicking Excess Electrons by Element Substitution. *ChemPlusChem*, **2012**, 77, 532-535	2.8	15
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