Nicola Gaston

List of Publications by Year
in descending order

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76 papers	1,677 citations	304743 22 h-index	315739 38 g-index
79 all docs	79 docs citations	79 times ranked	2232 citing authors

#	Article	IF	Citations
1	Oscillatory bifurcation patterns initiated by seeded surface solidification of liquid metals. , 2022, 1, 158-169.		15
2	Molecular crystals vs. superatomic lattice: a case study with superalkali-superhalogen compounds. Physical Chemistry Chemical Physics, 2022, 24, 8763-8774.	2.8	4
3	Catalytic Potential of Postâ€Transition Metal Doped Grapheneâ€Based Singleâ€Atom Catalysts for the CO₂ Electroreduction Reaction. ChemPhysChem, 2022, 23, .	2.1	6
4	Gallenene. , 2022, , 107-119.		0
5	Two-dimensional aluminium, gallium, and indium metallic crystals by first-principles design. Journal of Physics Condensed Matter, 2021, 33, 125901.	1.8	12
6	Unique surface patterns emerging during solidification of liquid metal alloys. Nature Nanotechnology, 2021, 16, 431-439.	31.5	104
7	Structural, Thermal, and Electronic Properties of Twoâ€Dimensional Gallium Oxide (Î²â€Ga₂O₃) from Firstâ€Principles Design. ChemPhysChem, 2021, 22, 2362-2370.	2.1	10
8	Emergent electronic properties in Co-deposited superatomic clusters. Journal of Chemical Physics, 2021, 155, 124309.	3.0	1
9	Modulating the thermal and structural stability of galleneneviavariation of atomistic thickness. Nanoscale Advances, 2021, 3, 499-507.	4.6	10
10	A mechanistic understanding of surface Bi enrichment in dilute GaBi systems. Physical Chemistry Chemical Physics, 2021, 23, 14383-14390.	2.8	2
11	Bimetallic superalkali substitution in the CsPbBr3 perovskite: Pseudocubic phases and tunable bandgap. Journal of Chemical Physics, 2021, 155, 174307.	3.0	6
12	Clustering of metal dopants in defect sites of graphene-based materials. Physical Chemistry Chemical Physics, 2021, 24, 98-111.	2.8	3
13	Bidirectional Control of the Band Bending at the (2Ì…01) and (010) Surfaces of Î²-Ga₂O₃ Using Aryldiazonium Ion and Phosphonic Acid Grafting. ACS Applied Electronic Materials, 2021, 3, 5608-5620.	4.3	4
14	On the influence of exact exchange on transition metal superatoms. Physical Chemistry Chemical Physics, 2020, 22, 772-780.	2.8	3
15	Ultra stable superatomic structure of doubly magic Ga₁₃ and Ga₁₃Li electrolyte. Nanoscale, 2020, 12, 289-295.	5.6	3
16	N4Mg6M (M = Li, Na, K) superalkalis for CO2 activation. Journal of Chemical Physics, 2020, 153, 144301.	3.0	15
17	Design of superatomic systems: exploiting favourable conditions for the delocalisation of d-electron density in transition metal doped clusters. Physical Chemistry Chemical Physics, 2020, 22, 18585-18594.	2.8	5
18	Modified Lennardâ€Jones potentials for nanoscale atoms. Journal of Computational Chemistry, 2020, 41, 1985-2000.	3.3	5

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19	5-Fold symmetry in superatomic scandium clusters: exploiting favourable orbital overlap to sequester spin. Physical Chemistry Chemical Physics, 2020, 22, 4051-4058.	2.8	5
20	Unveiling the structures and electronic properties of CH3NH3PbI3 interfaces with TiO2, ZnO, and SnO2: a first-principles study. Journal of Materials Science, 2019, 54, 13594-13608.	3.7	5
21	Internal and external pressure in cubic perovskites: electronic structure effects and systematic accuracy from first principles. Electronic Structure, 2019, 1, 035001.	2.8	6
22	Tuneable magnetic moments in superatomic Cu _X Ni _{8â^' X} clusters. Electronic Structure, 2019, 1, 035003.	2.8	2
23	Thickness dependent thermal stability of 2D gallenene. Chemical Communications, 2019, 55, 8872-8875.	4.1	19
24	On the involvement of d-electrons in superatomic shells: the group 3 and 4 transition metals. Physical Chemistry Chemical Physics, 2019, 21, 8035-8045.	2.8	11
25	Aluminum oxoâ€fluoride clusters: A first principle investigation of stability, synthetic considerations, and the interaction with water. Journal of Computational Chemistry, 2018, 39, 1208-1214.	3.3	2
26	Cluster melting: new, limiting, and liminal phenomena. Advances in Physics: X, 2018, 3, 1401487.	4.1	5
27	Shape-, Size-, and Composition-Controlled Thallium Lead Halide Perovskite Nanowires and Nanocrystals with Tunable Band Gaps. Chemistry of Materials, 2018, 30, 2973-2982.	6.7	28
28	Experimental and ab initio study of Mg doping in the intrinsic ferromagnetic semiconductor GdN. Journal of Applied Physics, 2018, 123, .	2.5	5
29	Cluster assemblies as superatomic solids: a first principles study of bonding & electronic structure. Physical Chemistry Chemical Physics, 2018, 20, 6167-6175.	2.8	8
30	How robust is the metallicity of two dimensional gallium?. Physical Chemistry Chemical Physics, 2018, 20, 27668-27674.	2.8	14
31	Building machine learning force fields for nanoclusters. Journal of Chemical Physics, 2018, 148, 241739.	3.0	42
32	The Evolution of Quantum Confinement in CsPbBr₃ Perovskite Nanocrystals. Chemistry of Materials, 2017, 29, 3644-3652.	6.7	258
33	Superatomic states in nickel clusters: Revising the prospects for transition metal based superatoms. Journal of Chemical Physics, 2017, 147, 154307.	3.0	8
34	Interaction of Boron Nitride Nanosheets with Model Cell Membranes. ChemPhysChem, 2016, 17, 1573-1578.	2.1	20
35	Phosphine passivated gold clusters: how charge transfer affects electronic structure and stability. Physical Chemistry Chemical Physics, 2016, 18, 29686-29697.	2.8	18
36	From the Superatom Model to a Diverse Array of Superâ€Elements: A Systematic Study of Dopant Influence on the Electronic Structure of Thiolateâ€Protected Gold Clusters. ChemPhysChem, 2016, 17, 3237-3244.	2.1	13

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37	First-principles calculations of the electronic structure and bonding in metal clusterâ€“fullerene materials considered within the superatomic framework. Physical Chemistry Chemical Physics, 2016, 18, 32541-32550.	2.8	12
38	A Two-Dimensional Liquid Structure Explains the Elevated Melting Temperatures of Gallium Nanoclusters. Nano Letters, 2016, 16, 21-26.	9.1	18
39	Hybrid density functional calculations of the surface electronic structure of GdN. Physical Review B, 2015, 91, .	3.2	1
40	Quantum Size Effects in the Sizeâ€“Temperature Phase Diagram of Gallium: Structural Characterization of Shapeâ€Shifting Clusters. Chemistry - A European Journal, 2015, 21, 2862-2869.	3.3	16
41	Al₂₀⁺does melt, albeit above the bulk melting temperature of aluminium. Physical Chemistry Chemical Physics, 2015, 17, 3741-3748.	2.8	10
42	Weak interactions in Graphane/BN systems under static electric fieldsâ€”A periodic ab-initio study. Journal of Chemical Physics, 2015, 142, 154701.	3.0	4
43	Characterizing the Greater-Than-Bulk Melting Behavior of Gaâ€“Al Nanoalloys. Journal of Physical Chemistry C, 2015, 119, 24095-24103.	3.1	3
44	Free up systems for funding and advice. Nature, 2014, 508, 44-44.	27.8	0
45	Method of increments for the halogen molecular crystals: Cl, Br, and I. Journal of Chemical Physics, 2014, 141, 124707.	3.0	13
46	Two worlds collide: Image analysis methods for quantifying structural variation in cluster molecular dynamics. Journal of Chemical Physics, 2014, 140, 064102.	3.0	8
47	The dimeric nature of bonding in gallium: from small clusters to the Î±-gallium phase. Physical Chemistry Chemical Physics, 2014, 16, 24244-24249.	2.8	17
48	A balanced procedure for the treatment of clusterâ€“ligand interactions on gold phosphine systems in catalysis. Journal of Computational Chemistry, 2014, 35, 986-997.	3.3	24
49	Câ€“Cl Bond Activation on Au/Pd Bimetallic Nanocatalysts Studied by Density Functional Theory and Genetic Algorithm Calculations. Journal of Physical Chemistry C, 2014, 118, 22188-22196.	3.1	39
50	Towards understanding the chemical environment effect on gold-containing clusters. Journal of Cheminformatics, 2014, 6, .	6.1	0
51	How a single aluminum atom makes a difference to gallium: First-principles simulations of bimetallic cluster melting. Journal of Chemical Physics, 2013, 139, 094309.	3.0	9
52	Interaction of Pyridine Derivatives with a Gold (111) Surface as a Model for Adsorption to Large Nanoparticles. Journal of Physical Chemistry C, 2013, 117, 4470-4479.	3.1	45
53	First-principles melting of gallium clusters down to nine atoms: structural and electronic contributions to melting. Physical Chemistry Chemical Physics, 2013, 15, 15325.	2.8	37
54	Geometrically induced melting variation in gallium clusters from first principles. Physical Review B, 2013, 88, .	3.2	17

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55	Electronic effects on the melting of small gallium clusters. Journal of Chemical Physics, 2012, 137, 144307.	3.0	30
56	Electronic shell structure in Ga12 icosahedra and the relation to the bulk forms of gallium. Physical Chemistry Chemical Physics, 2012, 14, 9912.	2.8	20
57	Extended X-ray Absorption Fine Structure and X-ray Diffraction Examination of Sputtered Nickel Carbon Binary Thin Films for Fuel Cell Applications. Journal of Physical Chemistry C, 2012, 116, 6159-6165.	3.1	10
58	Throwing jellium at galliumâ€"a systematic superatom analysis of metalloid gallium clusters. Physical Chemistry Chemical Physics, 2011, 13, 21109.	2.8	28
59	Synthesis and Comparison of the Magnetic Properties of Iron Sulfide Spinel and Iron Oxide Spinel Nanocrystals. Chemistry of Materials, 2011, 23, 2514-2517.	6.7	45
60	On the bonding of Ga2, structures of Gan clusters and the relation to the bulk structure of gallium. Chemical Physics Letters, 2011, 501, 375-378.	2.6	28
61	Understanding the hcp anisotropy in Cd and Zn: the role of electron correlation in determining the potential energy surface. Physical Chemistry Chemical Physics, 2010, 12, 681-687.	2.8	25
62	Hydrogen adsorption on model tungsten carbide surfaces. Catalysis Today, 2009, 146, 223-229.	4.4	29
63	EXAFS Analysis of Electrocatalytic WC Materials. Journal of Physical Chemistry C, 2009, 113, 17407-17410.	3.1	8
64	Multiple Minima on the Energy Landscape of Elemental Zinc: A Wave Function BasedAbÂInitioStudy. Physical Review Letters, 2008, 100, 226404.	7.8	35
65	Embedding procedure for ab initio correlation calculations in group II metals. Journal of Chemical Physics, 2007, 126, 134115.	3.0	42
66	Ab initiocorrelation calculations for the ground-state properties of group-12 metals Zn and Cd. Physical Review B, 2007, 76, .	3.2	22
67	Is Eka-Mercury (Element 112) a Group 12 Metal?. Angewandte Chemie - International Edition, 2007, 46, 1663-1666.	13.8	69
68	From the van der Waals dimer to the solid state of mercury with relativisticab initioand density functional theory. Physical Review B, 2006, 74, .	3.2	42
69	Extension of the Lennard-Jones potential: Theoretical investigations into rare-gas clusters and crystal lattices of He, Ne, Ar, and Kr using many-body interaction expansions. Physical Review B, 2006, 73, .	3.2	112
70	The frequency-dependent dipole polarizability of the mercury dimer from four-component relativistic density-functional theory. Journal of Chemical Physics, 2006, 124, 044304.	3.0	17
71	Photoabsorption spectra of cationic mercury clusters. Physical Review A, 2006, 74, .	2.5	9
72	Lattice structure of mercury: Influence of electronic correlation. Physical Review B, 2006, 74, .	3.2	57

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73	Ab initio Correlation Calculations for the Lattice Structures of Zn, Cd and Hg. , 2006, , 891-896.		0
74	Convergence of theab initiomany-body expansion for the cohesive energy of solid mercury. Physical Review B, 2004, 70, .	3.2	72
75	Ionization potentials of internal conversion electrons for the superheavy elements 112, 114, 116, and 118. Physical Review A, 2002, 66, .	2.5	21
76	Fairness and Equality in Research. ChemistryViews, 0, , .	0.0	0