Amanda Barnard

List of Publications by Citations

239 papers	8,374 citations	48 h-index	81 g-index
254 ext. papers	9,096 ext. citations	6.7 avg, IF	6.8 L-index

#	Paper	IF	Citations
239	Prediction of TiO2 nanoparticle phase and shape transitions controlled by surface chemistry. *Nano Letters*, **2005**, 5, 1261-6	11.5	556
238	Observation and control of blinking nitrogen-vacancy centres in discrete nanodiamonds. *Nature Nanotechnology*, **2010**, 5, 345-9	28.7	354
237	A model for the phase stability of arbitrary nanoparticles as a function of size and shape. *Journal of Chemical Physics*, **2004**, 121, 4276-83	3.9	234
236	Crystallinity and surface electrostatics of diamond nanocrystals. *Journal of Materials Chemistry*, **2007**, 17, 4811		199
235	Nanogold: a quantitative phase map. *ACS Nano*, **2009**, 3, 1431-6	16.7	197
234	Effects of particle morphology and surface hydrogenation on the phase stability of TiO2. *Physical Review B*, **2004**, 70,	3.3	191
233	Modeling the Morphology and Phase Stability of TiO2 Nanocrystals in Water. *Journal of Chemical Theory and Computation*, **2005**, 1, 107-16	6.4	183
232	Naturally occurring iron oxide nanoparticles: morphology, surface chemistry and environmental stability. *Journal of Materials Chemistry A*, **2013**, 1, 27-42	13	170
231	Modelling of nanoparticles: approaches to morphology and evolution. *Reports on Progress in Physics* , **2010**, 73, 086502	14.4	147
230	Self-assembly in nanodiamond agglutinates. *Journal of Materials Chemistry*, **2008**, 18, 4038		139
229	Equilibrium morphology of face-centered cubic gold nanoparticles >3 nm and the shape changes induced by temperature. *Journal of Physical Chemistry B*, **2005**, 109, 24465-72	3.4	131
228	Diamond standard in diagnostics: nanodiamond biolabels make their mark. *Analyst, The*, **2009**, 134, 1751-64	4	126
227	Shaping Nanometer-Scale Architecture Through Surface Chemistry. *Advanced Materials*, **2005**, 17, 965-971	21	122
226	Size, Shape, Stability, and Color of Plasmonic Silver Nanoparticles. *Journal of Physical Chemistry C*, **2014**, 118, 9128-9136	3.8	117
225	Confirmation of the electrostatic self-assembly of nanodiamonds. *Nanoscale*, **2011**, 3, 958-62	7.7	108
224	Nanodiamond Photoemitters Based on Strong Narrow-Band Luminescence from Silicon-Vacancy Defects. *Advanced Materials*, **2009**, 21, 808-812	24	108
223	Predicting the Energetics, Phase Stability, and Morphology Evolution of Faceted and Spherical Anatase Nanocrystals. *Journal of Physical Chemistry B*, **2004**, 108, 18435-18440	3.4	106

222	Anatase and rutile surfaces with adsorbates representative of acidic and basic conditions. *Surface Science*, **2005**, 582, 173-188	1.8	101
221	Structural relaxation and relative stability of nanodiamond morphologies. *Diamond and Related Materials*, **2003**, 12, 1867-1872	3.5	100
220	Coexistence of bucky diamond with nanodiamond and fullerene carbon phases. *Physical Review B*, **2003**, 68,	3.3	100
219	Atomistic simulation and measurement of pH dependent cancer therapeutic interactions with nanodiamond carrier. *Molecular Pharmaceutics*, **2011**, 8, 368-74	5.6	97
218	A thermodynamic model for the shape and stability of twinned nanostructures. *Journal of Physical Chemistry B*, **2006**, 110, 24498-504	3.4	97
217	Thermodynamic modelling of nanomorphologies of hematite and goethite. *Journal of Materials Chemistry*, **2011**, 21, 11566		95
216	Resolving the structure of active sites on platinum catalytic nanoparticles. *Nano Letters*, **2010**, 10, 3073-6	11.5	94
215	Towards chromate-free corrosion inhibitors: structure–property models for organic alternatives. *Green Chemistry*, **2014**, 16, 3349-3357	10	93
214	Prediction and measurement of the size-dependent stability of fluorescence in diamond over the entire nanoscale. *Nano Letters*, **2009**, 9, 3555-64	11.5	84
213	Size dependent phase stability of carbon nanoparticles: Nanodiamond versus fullerenes. *Journal of Chemical Physics*, **2003**, 118, 5094-5097	3.9	83
212	Structure and Energetics of Single-Walled Armchair and Zigzag Silicon Nanotubes. *Journal of Physical Chemistry B*, **2003**, 107, 7577-7581	3.4	79
211	An environmentally sensitive phase map of titania nanocrystals. *ACS Nano*, **2008**, 2, 2237-42	16.7	78
210	Nanohazards: knowledge is our first defence. *Nature Materials*, **2006**, 5, 245-8	27	76
209	One-to-one comparison of sunscreen efficacy, aesthetics and potential nanotoxicity. *Nature Nanotechnology*, **2010**, 5, 271-4	28.7	69
208	ZnO nanowires and nanobelts: Shape selection and thermodynamic modeling. *Applied Physics Letters*, **2007**, 90, 143116	3.4	69
207	Thermal stability of graphene edge structure and graphene nanoflakes. *Journal of Chemical Physics*, **2008**, 128, 094707	3.9	68
206	Predicting the shape and structure of face-centered cubic gold nanocrystals smaller than 3 nm. *ChemPhysChem*, **2006**, 7, 1544-53	3.2	68
205	Ab Initio Modeling of Diamond Nanowire Structures. *Nano Letters*, **2003**, 3, 1323-1328	11.5	68

204	Activity of ZnO polar surfaces: an insight from surface energies. *Physical Chemistry Chemical Physics*, **2014**, 16, 22139-44	3.6	67
203	Ab initio modelling of the stability of nanocrystalline diamond morphologies. *Philosophical Magazine Letters*, **2003**, 83, 39-45	1	63
202	Substitutional nitrogen in nanodiamond and bucky-diamond particles. *Journal of Physical Chemistry B*, **2005**, 109, 17107-12	3.4	62
201	Origin of nanomorphology: does a complete theory of nanoparticle evolution exist?. *Journal of Materials Chemistry*, **2010**, 20, 416-421		61
200	Direct comparison of kinetic and thermodynamic influences on gold nanomorphology. *Accounts of Chemical Research*, **2012**, 45, 1688-97	24.3	59
199	Geometrical Properties Can Predict CO2 and N2 Adsorption Performance of Metal-Organic Frameworks (MOFs) at Low Pressure. *ACS Combinatorial Science*, **2016**, 18, 243-52	3.9	59
198	Modeling the iron oxides and oxyhydroxides for the prediction of environmentally sensitive phase transformations. *Physical Review B*, **2011**, 83,	3.3	58
197	Three-Dimensional Branched and Faceted Gold-Ruthenium Nanoparticles: Using Nanostructure to Improve Stability in Oxygen Evolution Electrocatalysis. *Angewandte Chemie - International Edition*, **2018**, 57, 10241-10245	16.4	57
196	Modeling the thermostability of surface functionalisation by oxygen, hydroxyl, and water on nanodiamonds. *Nanoscale*, **2011**, 3, 2566-75	7.7	57
195	Controlled Evolution of Carbon Nanotubes Coated by Nanodiamond: the Realization of a New Class of Hybrid Nanomaterials. *Chemistry of Materials*, **2005**, 17, 3214-3220	9.6	57
194	Safe, stable and effective nanotechnology: phase mapping of ZnS nanoparticles. *Journal of Materials Chemistry*, **2010**, 20, 4971		54
193	Modeling the structure and electronic properties of TiO2 nanoparticles. *Physical Review B*, **2006**, 73,	3.3	52
192	Phase stability of nanocarbon in one dimension: nanotubes versus diamond nanowires. *Journal of Chemical Physics*, **2004**, 120, 3817-21	3.9	49
191	How can ab initio simulations address risks in nanotech?. *Nature Nanotechnology*, **2009**, 4, 332-5	28.7	48
190	Modelling the role of size, edge structure and terminations on the electronic properties of graphene nano-flakes. *Modelling and Simulation in Materials Science and Engineering*, **2011**, 19, 054001	2	47
189	Shape and Thermodynamic Stability of Pyrite FeS2Nanocrystals and Nanorods. *Journal of Physical Chemistry C*, **2007**, 111, 11742-11746	3.8	47
188	Modelling the effect of particle shape on the phase stability of ZrO2nanoparticles. *Nanotechnology*, **2006**, 17, 3039-3047	3.4	47
187	Machine Learning for Silver Nanoparticle Electron Transfer Property Prediction. *Journal of Chemical Information and Modeling*, **2017**, 57, 2413-2423	6.1	44

186	Substitutional boron in nanodiamond, bucky-diamond, and nanocrystalline diamond grain boundaries. *Journal of Physical Chemistry B*, **2006**, 110, 19307-14	3.4	44
185	First Principles and Thermodynamic Modeling of CdS Surfaces and Nanorods. *Journal of Physical Chemistry C*, **2007**, 111, 18112-18117	3.8	40
184	Stability of Nanodiamond Surfaces Exposed to N, NH, and NH2. *Journal of Physical Chemistry C*, **2011**, 115, 6218-6228	3.8	39
183	Harnessing the influence of reactive edges and defects of graphene substrates for achieving complete cycle of room-temperature molecular sensing. *Small*, **2013**, 9, 3993-9	11	38
182	Functionalized Nanodiamonds for Biological and Medical Applications. *Journal of Nanoscience and Nanotechnology*, **2015**, 15, 989-99	1.3	37
181	Electronic band gaps of diamond nanowires. *Physical Review B*, **2003**, 68,	3.3	37
180	Nanoinformatics, and the big challenges for the science of small things. *Nanoscale*, **2019**, 11, 19190-19201	7.7	36
179	Shape-Dependent Confinement of the Nanodiamond Band Gap. *Crystal Growth and Design*, **2009**, 9, 4860-4863	3.5	36
178	Modeling the preferred shape, orientation and aspect ratio of gold nanorods. *Journal of Materials Chemistry*, **2007**, 17, 3315		36
177	Interparticle Interactions and Self-Assembly of Functionalized Nanodiamonds. *Journal of Physical Chemistry Letters*, **2012**, 3, 896-901	6.4	35
176	Can we predict the location of impurities in diamond nanoparticles?. *Diamond and Related Materials* , **2007**, 16, 2078-2082	3.5	35
175	Using theory and modelling to investigate shape at the nanoscale. *Journal of Materials Chemistry*, **2006**, 16, 813-815		35
174	Modelling nanoscale FeS2 formation in sulfur rich conditions. *Journal of Materials Chemistry*, **2009**, 19, 3389		34
173	Predicting the distribution and stability of photoactive defect centers in nanodiamond biomarkers. *Journal of Materials Chemistry*, **2009**, 19, 360-365		33
172	Modelling the formation of high aspect CdSe quantum wires: axial-growth versus oriented-attachment mechanisms. *Nanotechnology*, **2006**, 17, 5707-14	3.4	33
171	Mapping the location and configuration of nitrogen in diamond nanoparticles. *Nanotechnology*, **2007**, 18, 025702	3.4	33
170	Theory and modeling of nanocarbon phase stability. *Diamond and Related Materials*, **2006**, 15, 285-291	3.5	31
169	Quantum mechanical properties of graphene nano-flakes and quantum dots. *Nanoscale*, **2012**, 4, 6761-7	7.7	30

168	Combining Theory and Experiment in Determining the Surface Chemistry of Nanocrystals. *Chemistry of Materials*, **2008**, 20, 5460-5463	9.6	30
167	Density Functional Study of H-Induced Defects as Nucleation Sites in Hybrid Carbon Nanomaterials. *Chemistry of Materials*, **2005**, 17, 527-535	9.6	30
166	Modeling of Stability and Phase Transformations in Quasi-Zero Dimensional Nanocarbon Systems. *Journal of Computational and Theoretical Nanoscience*, **2005**, 2, 180-201	0.3	30
165	The impact of structural polydispersivity on the surface electrostatic potential of nanodiamond. *Nanoscale*, **2014**, 6, 1188-94	7.7	29
164	Statistics, damned statistics and nanoscience - using data science to meet the challenge of nanomaterial complexity. *Nanoscale Horizons*, **2016**, 1, 89-95	10.8	28
163	Contrasting Effects of Nanoparticle Binding on Protein Denaturation. *Journal of Physical Chemistry C*, **2014**, 118, 22069-22078	3.8	28
162	Size- and shape-dependence of the graphene to graphane transformation in the absence of hydrogen. *Journal of Materials Chemistry*, **2010**, 20, 10459		28
161	Size dependent surface reconstruction in detonation nanodiamonds. *Nanoscale Horizons*, **2018**, 3, 213-217	10.8	27
160	Identification of Nanoparticle Prototypes and Archetypes. *ACS Nano*, **2015**, 9, 11980-92	16.7	26
159	Morphological and phase stability of zinc blende, amorphous and mixed core-shell ZnS nanoparticles. *Nanoscale*, **2010**, 2, 2294-301	7.7	26
158	Comparative Hartree-Fock and density-functional theory study of cubic and hexagonal diamond. *The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties*, **2002**, 82, 1767-1776		26
157	Geometrical features can predict electronic properties of graphene nanoflakes. *Carbon*, **2016**, 103, 142-150	6.0	25
156	Anisotropic adsorption and distribution of immobilized carboxyl on nanodiamond. *Nanoscale*, **2014**, 6, 14185-9	7.7	25
155	Modelling the role of size, edge structure and terminations on the electronic properties of trigonal graphene nanoflakes. *Nanotechnology*, **2012**, 23, 065707	3.4	25
154	Thermodynamic Cartography and Structure/Property Mapping of Commercial Platinum Catalysts. *ACS Catalysis*, **2011**, 1, 76-81	13.1	25
153	Transformation of graphene into graphane in the absence of hydrogen. *Carbon*, **2010**, 48, 981-986	10.4	25
152	Ab initio modelling of band states in doped diamond. *Philosophical Magazine*, **2003**, 83, 1163-1174	1.6	25
151	Counting vacancies and nitrogen-vacancy centers in detonation nanodiamond. *Nanoscale*, **2016**, 8, 10548-52	7.7	25

150	Can hematite nanoparticles be an environmental indicator?. *Energy and Environmental Science*, **2013**, 6, 561-569	35.4	24
149	Size- and shape-dependent phase transformations in wurtzite ZnS nanostructures. *Physical Chemistry Chemical Physics*, **2012**, 14, 9871-9	3.6	24
148	Morphology mapping of platinum catalysts over the entire nanoscale. *Catalysis Science and Technology*, **2011**, 1, 1440	5.5	24
147	Computational strategies for predicting the potential risks associated with nanotechnology. *Nanoscale*, **2009**, 1, 89-95	7.7	24
146	First Principles Investigations of Diamond Ultrananocrystals. *International Journal of Modern Physics B*, **2003**, 17, 3865-3879	1.1	24
145	Hydrogenation of Nanodiamond Surfaces: Structure and Effects on Crystalline Stability. *Surface Review and Letters*, **2003**, 10, 233-239	1.1	23
144	Development of an improved Stillinger-Weber potential for tetrahedral carbon using ab initio (Hartree-Fock and MP2) methods. *Molecular Physics*, **2002**, 100, 1517-1525	1.7	23
143	Morphology of Zinc Oxide Nanoparticles and Nanowires: Role of Surface and Edge Energies. *Journal of Physical Chemistry C*, **2016**, 120, 9498-9505	3.8	23
142	Surface phase diagram and thermodynamic stability of functionalisation of nanodiamonds. *Journal of Materials Chemistry*, **2012**, 22, 16774		22
141	Kinetic modelling of the shape-dependent evolution of faceted gold nanoparticles. *Journal of Materials Chemistry*, **2011**, 21, 12239		22
140	Machine Learning Prediction of the Energy Gap of Graphene Nanoflakes Using Topological Autocorrelation Vectors. *ACS Combinatorial Science*, **2016**, 18, 661-664	3.9	22
139	Surface structure of cubic diamond nanowires. *Surface Science*, **2003**, 538, 204-210	1.8	21
138	Understanding and Predicting the Cause of Defects in Graphene Oxide Nanostructures Using Machine Learning. *Journal of Physical Chemistry C*, **2020**, 124, 7404-7413	3.8	20
137	High throughput theory and simulation of nanomaterials: exploring the stability and electronic properties of nanographene. *Journal of Materials Chemistry*, **2012**, 22, 18119		20
136	Map of the Structural and Optical Properties of Gold Nanoparticles at Thermal Equilibrium. *Journal of Physical Chemistry C*, **2012**, 116, 14170-14175	3.8	20
135	Modelling the shape and orientation of ZnO nanobelts. *Chemical Physics Letters*, **2006**, 419, 313-316	2.5	20
134	From nanodiamond to diamond nanowires: structural properties affected by dimension. *Philosophical Magazine*, **2004**, 84, 899-907	1.6	20
133	Ab initio modeling of B and N in C29 and C29H24 nanodiamond. *Journal of Chemical Physics*, **2003**, 118, 10725-10728	3.9	20

132	Predicting the impact of structural diversity on the performance of nanodiamond drug carriers. *Nanoscale*, **2018**, 10, 8893-8910	7.7	19
131	Dynamic evolution of specific catalytic sites on Pt nanoparticles. *Catalysis Science and Technology*, **2016**, 6, 144-151	5.5	19
130	Selecting Appropriate Clustering Methods for Materials Science Applications of Machine Learning. *Advanced Theory and Simulations*, **2019**, 2, 1900145	3.5	19
129	Quantitative Structure-Property Relationship Modeling of Electronic Properties of Graphene Using Atomic Radial Distribution Function Scores. *Journal of Chemical Information and Modeling*, **2015**, 55, 2500-6	6.1	19
128	Nanodiamond for hydrogen storage: temperature-dependent hydrogenation and charge-induced dehydrogenation. *Nanoscale*, **2012**, 4, 1130-7	7.7	19
127	Environmentally dependent stability of low-index hematite surfaces. *Journal of Colloid and Interface Science*, **2012**, 386, 315-24	9.3	19
126	Surface Area Limited Model for Predicting Anisotropic Coarsening of Faceted Nanoparticles. *Crystal Growth and Design*, **2011**, 11, 158-165	3.5	19
125	Vacancy Induced Structural Changes in Diamond Nanoparticles. *Journal of Computational and Theoretical Nanoscience*, **2008**, 5, 2089-2095	0.3	19
124	Artificial neural network analysis of the catalytic efficiency of platinum nanoparticles. *RSC Advances* , **2017**, 7, 48962-48971	3.7	18
123	Mapping the shape and phase of palladium nanocatalysts. *Catalysis Science and Technology*, **2012**, 2, 1485	5.5	18
122	Modeling polydispersive ensembles of diamond nanoparticles. *Nanotechnology*, **2013**, 24, 085703	3.4	18
121	Surface Structure and Environment-Dependent Hydroxylation of the Nonpolar Hematite (100) from Density Functional Theory Modeling. *Journal of Physical Chemistry C*, **2011**, 115, 23023-23029	3.8	18
120	Shape dependence of the band gaps in luminescent silicon quantum dots. *Journal of Materials Chemistry C*, **2014**, 2, 9451-9456	7.1	17
119	Clarifying stability, probability and population in nanoparticle ensembles. *Nanoscale*, **2014**, 6, 9983-90	7.7	17
118	Size and shape dependent deprotonation potential and proton affinity of nanodiamond. *Nanotechnology*, **2014**, 25, 445702	3.4	16
117	Ripple induced changes in the wavefunction of graphene: an example of a fundamental symmetry breaking. *Nanoscale*, **2012**, 4, 1167-70	7.7	16
116	Thermodynamic stability and electronic structure of small carbon nitride nanotubes. *Journal of Physics Condensed Matter*, **2009**, 21, 144203	1.8	16
115	Morphological Stability of Pyrite FeS2 Nanocrystals in Water. *Journal of Physical Chemistry C*, **2009**, 113, 5376-5380	3.8	16

114	Visualising multi-dimensional structure/property relationships with machine learning. *JPhys Materials*, **2019**, 2, 034003	4.2	15
113	Using structural diversity to tune the catalytic performance of Pt nanoparticle ensembles. *Catalysis Science and Technology*, **2015**, 5, 2848-2855	5.5	15
112	Molecular ionization and deprotonation energies as indicators of functional coating performance. *Journal of Materials Chemistry A*, **2014**, 2, 16660-16668	13	15
111	Shape, Orientation, and Stability of Twinned Gold Nanorods. *Journal of Physical Chemistry C*, **2008**, 112, 1385-1390	3.8	15
110	Bucky-wires and the instability of diamond (111) surfaces in one-dimension. *Journal of Nanoscience and Nanotechnology*, **2004**, 4, 151-6	1.3	15
109	The representative structure of graphene oxide nanoflakes from machine learning. *Nano Futures*, **2019**, 3, 045001	3.6	15
108	Representing molecular and materials data for unsupervised machine learning. *Molecular Simulation*, **2018**, 44, 905-920	2	14
107	The impact of size and shape distributions on the electron charge transfer properties of silver nanoparticles. *Nanoscale*, **2017**, 9, 12698-12708	7.7	14
106	Relative Stability of Graphene Nanoflakes Under Environmentally Relevant Conditions. *Journal of Physical Chemistry C*, **2013**, 117, 15375-15382	3.8	14
105	Predicting structure/property relationships in multi-dimensional nanoparticle data using t-distributed stochastic neighbour embedding and machine learning. *Nanoscale*, **2019**, 11, 23165-23172	7.7	14
104	Materials science: nanoscale locomotion without fuel. *Nature*, **2015**, 519, 37-8	50.4	13
103	Dynamic self-assembly of detonation nanodiamond in water. *Nanoscale*, **2020**, 12, 5363-5367	7.7	13
102	Challenges in modelling nanoparticles for drug delivery. *Journal of Physics Condensed Matter*, **2016**, 28, 023002	1.8	13
101	Modeling the Impact of Alkanethiol SAMs on the Morphology of Gold Nanocrystals. *Crystal Growth and Design*, **2013**, 13, 5433-5441	3.5	13
100	Site-dependent stability and electronic structure of single vacancy point defects in hexagonal graphene nano-flakes. *Physical Chemistry Chemical Physics*, **2013**, 15, 4897-905	3.6	13
99	Modelling of the reactivity and stability of carbon nanotubes under environmentally relevant conditions. *Physical Chemistry Chemical Physics*, **2012**, 14, 10080-93	3.6	13
98	Useful equations for modeling the relative stability of common nanoparticle morphologies. *Computer Physics Communications*, **2011**, 182, 11-13	4.2	13
97	Classification of platinum nanoparticle catalysts using machine learning. *Journal of Applied Physics*, **2020**, 128, 014301	2.5	13

96	Thermodynamics of Hydrogen Adsorption and Incorporation at the ZnO(101 0) Surface. *Journal of Physical Chemistry C*, **2015**, 119, 26560-26565	3.8	12
95	Impact of distributions and mixtures on the charge transfer properties of graphene nanoflakes. *Nanoscale*, **2015**, 7, 1864-71	7.7	12
94	Stability of Porous Platinum Nanoparticles: Combined In Situ TEM and Theoretical Study. *Journal of Physical Chemistry Letters*, **2012**, 3, 1106-10	6.4	12
93	From Process to Properties: Correlating Synthesis Conditions and Structural Disorder of Platinum Nanocatalysts. *Journal of Physical Chemistry C*, **2018**, 122, 28085-28093	3.8	12
92	Towards developing multiscale-multiphysics models and their surrogates for digital twins of metal additive manufacturing. *Additive Manufacturing*, **2021**, 46, 102089	6.1	12
91	Efficient protocol for quantum Monte Carlo calculations of hydrogen abstraction barriers: Application to methanol. *International Journal of Quantum Chemistry*, **2017**, 117, e25361	2.1	11
90	Predictive Morphology Control of Hydrogen-Terminated Silicon Nanoparticles. *Journal of Physical Chemistry C*, **2014**, 118, 2580-2586	3.8	11
89	Tuning the Electron Transfer Properties of Entire Nanodiamond Ensembles. *Journal of Physical Chemistry C*, **2014**, 118, 30209-30215	3.8	11
88	Surface phase diagram of hematite pseudocubes in hydrous environments. *Journal of Materials Chemistry*, **2012**, 22, 161-167		11
87	Creation and luminescence of size-selected gold nanorods. *Nanoscale*, **2012**, 4, 5017-22	7.7	11
86	Mapping the structural and optical properties of anisotropic gold nanoparticles. *Journal of Materials Chemistry C*, **2013**, 1, 3150	7.1	11
85	Bonding and structure in BxNy nanotubes (x,y = 1,2). *Journal of Materials Chemistry*, **2007**, 17, 2892		11
84	First-principles modeling of dopants in C29 and C29H24 nanodiamonds. *Journal of Physical Chemistry B*, **2005**, 109, 11991-5	3.4	11
83	Classifying and predicting the electron affinity of diamond nanoparticles using machine learning. *Nanoscale Horizons*, **2019**, 4, 983-990	10.8	10
82	Optical Emission of Statistical Distributions of Silicon Quantum Dots. *Journal of Physical Chemistry C*, **2015**, 119, 7969-7977	3.8	10
81	Selecting machine learning models for metallic nanoparticles. *Nano Futures*, **2020**, 4, 035003	3.6	10
80	In silico veritas. *ACS Nano*, **2014**, 8, 6520-5	16.7	10
79	Machine learning and genetic algorithm prediction of energy differences between electronic calculations of graphene nanoflakes. *Nanotechnology*, **2017**, 28, 38LT03	3.4	10

78	Mapping the photocatalytic activity or potential free radical toxicity of nanoscale titania. *Energy and Environmental Science*, **2011**, 4, 439-443	35.4	10
77	Ideality versus Reality: Emergence of the Chui Icosahedron. *Journal of Physical Chemistry C*, **2008**, 112, 14848-14852	3.8	10
76	Hybrid carbon nanotube/nanodiamond structures as electron emitters for cold cathodes. *Journal of Nanoscience and Nanotechnology*, **2008**, 8, 1989-93	1.3	10
75	Shape and Energetics of TiN Nanoparticles. *Journal of Computational and Theoretical Nanoscience*, **2004**, 1, 334-339	0.3	10
74	Impact of distributions on the archetypes and prototypes in heterogeneous nanoparticle ensembles. *Nanoscale*, **2017**, 9, 832-843	7.7	9
73	Optimal vacancy concentrations to maximize the NV yield in nanodiamonds. *Materials Horizons*, **2014**, 1, 286	14.4	9
72	Ideality versus Reality: Predicting the Effect of Realistic Environments on the Electronic Properties of Nanographene. *Nanoscience and Nanotechnology Letters*, **2011**, 3, 59-62	0.8	9
71	Modeling corrosion inhibition efficacy of small organic molecules as non-toxic chromate alternatives using comparative molecular surface analysis (CoMSA). *Chemosphere*, **2016**, 160, 80-8	8.4	9
70	Predicting the role of seed morphology in the evolution of anisotropic nanocatalysts. *Nanoscale*, **2017**, 9, 1502-1510	7.7	8
69	Impact of distributions on the photocatalytic performance of anatase nanoparticle ensembles. *Journal of Materials Chemistry A*, **2015**, 3, 60-64	13	8
68	Phenol-Modified Silicene: Preferred Substitution Site and Electronic Properties. *Journal of Physical Chemistry C*, **2016**, 120, 6762-6770	3.8	8
67	Site-dependent atomic and molecular affinities of hydrocarbons, amines and thiols on diamond nanoparticles. *Nanoscale*, **2016**, 8, 7899-905	7.7	8
66	Technology: Sharing data in materials science. *Nature*, **2013**, 503, 463-4	50.4	8
65	Machine learning reveals multiple classes of diamond nanoparticles. *Nanoscale Horizons*, **2020**, 5, 1394-1398	10.8	8
64	Impact of speciation on the electron charge transfer properties of nanodiamond drug carriers. *Nanoscale*, **2016**, 8, 14264-70	7.7	8
63	PorosityPlus: characterisation of defective, nanoporous and amorphous materials. *JPhys Materials*, **2018**, 1, 016002	4.2	8
62	Predicting archetypal nanoparticle shapes using a combination of thermodynamic theory and machine learning. *Nanoscale*, **2018**, 10, 21818-21826	7.7	8
61	On reverse Monte Carlo constraints and model reproduction. *Journal of Computational Chemistry*, **2017**, 38, 1547-1551	3.5	7

60	Heterogeneous PEGylation of diamond nanoparticles. *Nanoscale*, **2017**, 9, 70-74	7.7	7
59	Does Twinning Impact Structure/Property Relationships in Diamond Nanoparticles?. *Journal of Physical Chemistry C*, **2019**, 123, 11207-11215	3.8	7
58	Accurate prediction of binding energies for two-dimensional catalytic materials using machine learning. *ChemCatChem*, **2020**, 12, 5109-5120	5.2	7
57	Thermodynamic Control of Halogen-Terminated Silicon Nanoparticle Morphology. *Crystal Growth and Design*, **2014**, 14, 4468-4474	3.5	7
56	Diamond nanoparticles as a new platform for the sequestration of waste carbon. *Physical Chemistry Chemical Physics*, **2013**, 15, 9156-62	3.6	7
55	Modelling polar wurtzite ZnS nanoparticles: the effect of sulphur supersaturation on size- and shape-dependent phase transformations. *Journal of Materials Chemistry*, **2012**, 22, 18992		7
54	Proton transfer in the hydrogen-bonded chains of lepidocrocite: a computational study. *Physical Chemistry Chemical Physics*, **2011**, 13, 17864-9	3.6	7
53	A comparative density functional theory investigation of the mechanical and energetic properties of ZnS. *Molecular Simulation*, **2011**, 37, 321-333	2	7
52	Ab initio modelling of boron and nitrogen in diamond nanowires. *Philosophical Magazine*, **2003**, 83, 2301-2309	1.8	7
51	The pure and representative types of disordered platinum nanoparticles from machine learning. *Nanotechnology*, **2021**, 32, 095404	3.4	7
50	Catalytic potential of highly defective (211) surfaces of zinc blende ZnO. *Physical Chemistry Chemical Physics*, **2015**, 17, 27683-9	3.6	6
49	Best Practice Leads to the Best Materials Informatics. *Matter*, **2020**, 3, 22-23	12.7	6
48	Bias-Free Chemically Diverse Test Sets from Machine Learning. *ACS Combinatorial Science*, **2017**, 19, 544-554	3.9	6
47	Modelling nanoscale cubic ZnS morphology and thermodynamic stability under sulphur-rich conditions. *CrystEngComm*, **2012**, 14, 7749	3.3	6
46	Modeling the environmental stability of FeS2 nanorods, using lessons from biomineralization. *Nanotechnology*, **2009**, 20, 115702	3.4	6
45	Characterization of cathodic arc deposited titanium aluminium nitride films prepared using plasma immersion ion implantation. *Journal of Physics Condensed Matter*, **2005**, 17, 2791-2800	1.8	6
44	Stability of Nanodiamond **2006**, 117-154		6
43	Carbon Family at the Nanoscale **2006**, 3-22		6

42	The data-intensive scientific revolution occurring where two-dimensional materials meet machine learning. *Cell Reports Physical Science*, **2021**, 2, 100482	6.1	6
41	Simulating nano-carbon materials. *Molecular Simulation*, **2005**, 31, 495-504	2	5
40	A Monte Carlo Study of Surface Reconstruction in (100) and (111) Diamond Surfaces and Nanodiamond. *Molecular Simulation*, **2004**, 30, 1-8	2	5
39	Simulation and bonding of dopants in nanocrystalline diamond. *Journal of Nanoscience and Nanotechnology*, **2005**, 5, 1395-407	1.3	5
38	Nearest neighbour considerations in Stillinger-Weber type potentials for diamond. *Molecular Simulation*, **2002**, 28, 761-771	2	5
37	Vacancy induced formation of nanoporous silicon, carbon and silicon carbide. *Physical Chemistry Chemical Physics*, **2019**, 21, 6517-6524	3.6	5
36	Correlating anisotropy and disorder with the surface structure of platinum nanoparticles. *Nanoscale*, **2018**, 10, 20393-20404	7.7	5
35	Charge-induced restructuring and decomposition of bucky-diamonds. *Journal of Materials Chemistry*, **2012**, 22, 13141		4
34	Ab initio modelling of dopants in diamond nanowires: Ii. *Philosophical Magazine*, **2003**, 83, 2311-2321	1.6	4
33	Water bilayers on ZnO(100) surfaces: data-driven structural search. *RSC Advances*, **2016**, 6, 30928-30936	3.7	4
32	Tunable charge transfer on selectively functionalised diamond nanoparticles. *Diamond and Related Materials*, **2016**, 68, 78-83	3.5	4
31	Fast derivation of Shapley based feature importances through feature extraction methods for nanoinformatics. *Machine Learning: Science and Technology*, **2021**, 2, 035034	5.1	4
30	Texture based image classification for nanoparticle surface characterisation and machine learning. *JPhys Materials*, **2018**, 1, 016001	4.2	3
29	Interfacial informatics. *JPhys Materials*, **2021**, 4, 041001	4.2	3
28	Identifying hidden high-dimensional structure/property relationships using self-organizing maps. *MRS Communications*, **2019**, 9, 730-736	2.7	2
27	Simulated nanoparticle assembly using protoparticles (SNAP). *JPhys Materials*, **2020**, 3, 026001	4.2	2
26	Feature Engineering of Solid-State Crystalline Lattices for Machine Learning. *Advanced Theory and Simulations*, **2020**, 3, 1900190	3.5	2
25	Atomic and Electronic Structures of Functionalized Nanodiamond Particles. *Microscopy and Microanalysis*, **2017**, 23, 2270-2271	0.5	2

24	Design of Nanodiamond Based Drug Delivery Patch for Cancer Therapeutics and Imaging Applications **2010**, 249-284		2
23	Modelling the relative stability of carbon nanotubes exposed to environmental adsorbates and air. *Journal of Physics Condensed Matter*, **2009**, 21, 144205	1.8	2
22	Partnerships for sustainable nanotechnology. *Materials Today*, **2009**, 12, 47	21.8	2
21	Thermodynamic Modeling of Hydrogen Adsorption on Carbon Nanotubes During CVD Growth. *Chemical Vapor Deposition*, **2006**, 12, 388-394		2
20	Simulating facet-dependent aggregation and assembly of distributions of polyhedral nanoparticles. *Nanoscale*, **2020**, 12, 19870-19879	7.7	2
19	Using hypothetical product configurators to measure consumer preferences for nanoparticle size and concentration in sunscreens. *Design Science*, **2016**, 2,	2.8	2
18	Impact of atomistic or crystallographic descriptors for classification of gold nanoparticles. *Nanoscale*, **2021**, 13, 11887-11898	7.7	2
17	Unsupervised structure classes vs. supervised property classes of silicon quantum dots using neural networks. *Nanoscale Horizons*, **2021**, 6, 277-282	10.8	2
16	Inverse Design of Nanoparticles Using Multi-Target Machine Learning. *Advanced Theory and Simulations*, **2022**, 5, 2100414	3.5	2
15	High-throughput simulation of the configuration and ionisation potential of nitrogen-doped graphene. *Molecular Simulation*, **2016**, 42, 458-462	2	1
14	Surface and Point Defect Measurements of Detonation Nanodiamond using Combined Cs-Cc corrected TEM and ab initio Calculations. *Microscopy and Microanalysis*, **2016**, 22, 1392-1393	0.5	1
13	Modeling Nanomorphology in Noble Metal Particles: Thermodynamic Cartography **2012**, 269-303		1
12	Stability of Diamond at the Nanoscale **2012**, 3-52		1
11	Hydrogen Stabilization of {111} Nanodiamond. *Materials Research Society Symposia Proceedings*, **2002**, 740, 1		1
10	Explainable prediction of N-V-related defects in nanodiamond using neural networks and Shapley values. *Cell Reports Physical Science*, **2022**, 3, 100696	6.1	1
9	Data-driven causal inference of process-structure relationships in nanocatalysis. *Current Opinion in Chemical Engineering*, **2022**, 36, 100818	5.4	1
8	Thermodynamics of Iron Oxides and Oxyhydroxides in Different Environments **2016**, 269-292		0
7	Simulating Facet-Dependent Aggregation and Assembly of Mixtures of Polyhedral Nanoparticles. *Advanced Theory and Simulations*,2100279	3.5	0

6	Charge-dependent Fermi level of graphene oxide nanoflakes from machine learning. *Computational Materials Science*, **2022**, 211, 111526	3.2	0
5	Safety-by-design using forward and inverse multi-target machine learning. *Chemosphere*, **2022**, 303, 135033	8.1	0
4	Optimization-Free Inverse Design of High-Dimensional Nanoparticle Electrocatalysts Using Multi-target Machine Learning. *Lecture Notes in Computer Science*, **2022**, 307-318	0.9	0
3	Aggregation Behavior of Detonation Nanodiamond in Solution. *Microscopy and Microanalysis*, **2019**, 25, 1740-1741	0.5	
2	Molecular and Analytical Modeling of Nanodiamond for Drug Delivery Applications **2015**, 169-195		
1	Predicting the Probability of Observation of Arbitrary Graphene Oxide Nanoflakes Using Artificial Neural Networks. *Advanced Theory and Simulations*,2200013	3.5	