Amanda Barnard

List of Publications by Year in Descending Order

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	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
238	Inverse Design of Nanoparticles Using Multi-Target Machine Learning. *Advanced Theory and Simulations*, **2022**, 5, 2100414	3.5	2
237	Data-driven causal inference of process-structure relationships in nanocatalysis. *Current Opinion in Chemical Engineering*, **2022**, 36, 100818	5.4	1
236	Charge-dependent Fermi level of graphene oxide nanoflakes from machine learning. *Computational Materials Science*, **2022**, 211, 111526	3.2	0
235	Safety-by-design using forward and inverse multi-target machine learning. *Chemosphere*, **2022**, 303, 135033	8.1	0
234	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
233	The pure and representative types of disordered platinum nanoparticles from machine learning. *Nanotechnology*, **2021**, 32, 095404	3.4	7
232	Impact of atomistic or crystallographic descriptors for classification of gold nanoparticles. *Nanoscale*, **2021**, 13, 11887-11898	7.7	2
231	Unsupervised structure classes vs. supervised property classes of silicon quantum dots using neural networks. *Nanoscale Horizons*, **2021**, 6, 277-282	10.8	2
230	Interfacial informatics. *JPhys Materials*, **2021**, 4, 041001	4.2	3
229	The data-intensive scientific revolution occurring where two-dimensional materials meet machine learning. *Cell Reports Physical Science*, **2021**, 2, 100482	6.1	6
228	Fast derivation of Shapley based feature importances through feature extraction methods for nanoinformatics. *Machine Learning: Science and Technology*, **2021**, 2, 035034	5.1	4
227	Towards developing multiscale-multiphysics models and their surrogates for digital twins of metal additive manufacturing. *Additive Manufacturing*, **2021**, 46, 102089	6.1	12
226	Accurate prediction of binding energies for two-dimensional catalytic materials using machine learning. *ChemCatChem*, **2020**, 12, 5109-5120	5.2	7
225	Selecting machine learning models for metallic nanoparticles. *Nano Futures*, **2020**, 4, 035003	3.6	10
224	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
223	Best Practice Leads to the Best Materials Informatics. *Matter*, **2020**, 3, 22-23	12.7	6

222	Simulated nanoparticle assembly using protoparticles (SNAP). *JPhys Materials*, **2020**, 3, 026001	4.2	2
221	Dynamic self-assembly of detonation nanodiamond in water. *Nanoscale*, **2020**, 12, 5363-5367	7.7	13
220	Feature Engineering of Solid-State Crystalline Lattices for Machine Learning. *Advanced Theory and Simulations*, **2020**, 3, 1900190	3.5	2
219	Classification of platinum nanoparticle catalysts using machine learning. *Journal of Applied Physics*, **2020**, 128, 014301	2.5	13
218	Machine learning reveals multiple classes of diamond nanoparticles. *Nanoscale Horizons*, **2020**, 5, 1394-1398	8.8	8
217	Simulating facet-dependent aggregation and assembly of distributions of polyhedral nanoparticles. *Nanoscale*, **2020**, 12, 19870-19879	7.7	2
216	Identifying hidden high-dimensional structure/property relationships using self-organizing maps. *MRS Communications*, **2019**, 9, 730-736	2.7	2
215	Does Twinning Impact Structure/Property Relationships in Diamond Nanoparticles?. *Journal of Physical Chemistry C*, **2019**, 123, 11207-11215	3.8	7
214	Classifying and predicting the electron affinity of diamond nanoparticles using machine learning. *Nanoscale Horizons*, **2019**, 4, 983-990	10.8	10
213	Visualising multi-dimensional structure/property relationships with machine learning. *JPhys Materials*, **2019**, 2, 034003	4.2	15
212	Nanoinformatics, and the big challenges for the science of small things. *Nanoscale*, **2019**, 11, 19190-19201	7.7	36
211	Aggregation Behavior of Detonation Nanodiamond in Solution. *Microscopy and Microanalysis*, **2019**, 25, 1740-1741	0.5	
210	Selecting Appropriate Clustering Methods for Materials Science Applications of Machine Learning. *Advanced Theory and Simulations*, **2019**, 2, 1900145	3.5	19
209	Vacancy induced formation of nanoporous silicon, carbon and silicon carbide. *Physical Chemistry Chemical Physics*, **2019**, 21, 6517-6524	3.6	5
208	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
207	The representative structure of graphene oxide nanoflakes from machine learning. *Nano Futures*, **2019**, 3, 045001	3.6	15
206	Predicting the impact of structural diversity on the performance of nanodiamond drug carriers. *Nanoscale*, **2018**, 10, 8893-8910	7.7	19
205	Representing molecular and materials data for unsupervised machine learning. *Molecular Simulation*, **2018**, 44, 905-920	2	14

204	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
203	Size dependent surface reconstruction in detonation nanodiamonds. *Nanoscale Horizons*, **2018**, 3, 213-217	6.8	27
202	PorosityPlus: characterisation of defective, nanoporous and amorphous materials. *JPhys Materials*, **2018**, 1, 016002	4.2	8
201	Texture based image classification for nanoparticle surface characterisation and machine learning. *JPhys Materials*, **2018**, 1, 016001	4.2	3
200	Predicting archetypal nanoparticle shapes using a combination of thermodynamic theory and machine learning. *Nanoscale*, **2018**, 10, 21818-21826	7.7	8
199	Correlating anisotropy and disorder with the surface structure of platinum nanoparticles. *Nanoscale*, **2018**, 10, 20393-20404	7.7	5
198	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
197	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
196	On reverse Monte Carlo constraints and model reproduction. *Journal of Computational Chemistry*, **2017**, 38, 1547-1551	3.5	7
195	Heterogeneous PEGylation of diamond nanoparticles. *Nanoscale*, **2017**, 9, 70-74	7.7	7
194	Impact of distributions on the archetypes and prototypes in heterogeneous nanoparticle ensembles. *Nanoscale*, **2017**, 9, 832-843	7.7	9
193	Predicting the role of seed morphology in the evolution of anisotropic nanocatalysts. *Nanoscale*, **2017**, 9, 1502-1510	7.7	8
192	Machine Learning for Silver Nanoparticle Electron Transfer Property Prediction. *Journal of Chemical Information and Modeling*, **2017**, 57, 2413-2423	6.1	44
191	Artificial neural network analysis of the catalytic efficiency of platinum nanoparticles. *RSC Advances* , **2017**, 7, 48962-48971	3.7	18
190	Atomic and Electronic Structures of Functionalized Nanodiamond Particles. *Microscopy and Microanalysis*, **2017**, 23, 2270-2271	0.5	2
189	The impact of size and shape distributions on the electron charge transfer properties of silver nanoparticles. *Nanoscale*, **2017**, 9, 12698-12708	7.7	14
188	Bias-Free Chemically Diverse Test Sets from Machine Learning. *ACS Combinatorial Science*, **2017**, 19, 544-554	3.9	6
187	Machine learning and genetic algorithm prediction of energy differences between electronic calculations of graphene nanoflakes. *Nanotechnology*, **2017**, 28, 38LT03	3.4	10

186	High-throughput simulation of the configuration and ionisation potential of nitrogen-doped graphene. *Molecular Simulation*, **2016**, 42, 458-462	2	1
185	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
184	Thermodynamics of Iron Oxides and Oxyhydroxides in Different Environments **2016**, 269-292		0
183	Phenol-Modified Silicene: Preferred Substitution Site and Electronic Properties. *Journal of Physical Chemistry C*, **2016**, 120, 6762-6770	3.8	8
182	Site-dependent atomic and molecular affinities of hydrocarbons, amines and thiols on diamond nanoparticles. *Nanoscale*, **2016**, 8, 7899-905	7.7	8
181	Geometrical features can predict electronic properties of graphene nanoflakes. *Carbon*, **2016**, 103, 142-150	6.2	25
180	Statistics, damned statistics and nanoscience - using data science to meet the challenge of nanomaterial complexity. *Nanoscale Horizons*, **2016**, 1, 89-95	10.8	28
179	Challenges in modelling nanoparticles for drug delivery. *Journal of Physics Condensed Matter*, **2016**, 28, 023002	1.8	13
178	Dynamic evolution of specific catalytic sites on Pt nanoparticles. *Catalysis Science and Technology*, **2016**, 6, 144-151	5.5	19
177	Using hypothetical product configurators to measure consumer preferences for nanoparticle size and concentration in sunscreens. *Design Science*, **2016**, 2,	2.8	2
176	Impact of speciation on the electron charge transfer properties of nanodiamond drug carriers. *Nanoscale*, **2016**, 8, 14264-70	7.7	8
175	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
174	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
173	Water bilayers on ZnO(100) surfaces: data-driven structural search. *RSC Advances*, **2016**, 6, 30928-30936	3.7	4
172	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
171	Counting vacancies and nitrogen-vacancy centers in detonation nanodiamond. *Nanoscale*, **2016**, 8, 10548-52	7.7	25
170	Tunable charge transfer on selectively functionalised diamond nanoparticles. *Diamond and Related Materials*, **2016**, 68, 78-83	3.5	4
169	Machine Learning Prediction of the Energy Gap of Graphene Nanoflakes Using Topological Autocorrelation Vectors. *ACS Combinatorial Science*, **2016**, 18, 661-664	3.9	22

168	Using structural diversity to tune the catalytic performance of Pt nanoparticle ensembles. *Catalysis Science and Technology*, **2015**, 5, 2848-2855	5.5	15
167	Materials science: nanoscale locomotion without fuel. *Nature*, **2015**, 519, 37-8	50.4	13
166	Optical Emission of Statistical Distributions of Silicon Quantum Dots. *Journal of Physical Chemistry C*, **2015**, 119, 7969-7977	3.8	10
165	Catalytic potential of highly defective (211) surfaces of zinc blende ZnO. *Physical Chemistry Chemical Physics*, **2015**, 17, 27683-9	3.6	6
164	Impact of distributions on the photocatalytic performance of anatase nanoparticle ensembles. *Journal of Materials Chemistry A*, **2015**, 3, 60-64	13	8
163	Thermodynamics of Hydrogen Adsorption and Incorporation at the ZnO(101 0) Surface. *Journal of Physical Chemistry C*, **2015**, 119, 26560-26565	3.8	12
162	Identification of Nanoparticle Prototypes and Archetypes. *ACS Nano*, **2015**, 9, 11980-92	16.7	26
161	Impact of distributions and mixtures on the charge transfer properties of graphene nanoflakes. *Nanoscale*, **2015**, 7, 1864-71	7.7	12
160	Molecular and Analytical Modeling of Nanodiamond for Drug Delivery Applications **2015**, 169-195		
159	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
158	Functionalized Nanodiamonds for Biological and Medical Applications. *Journal of Nanoscience and Nanotechnology*, **2015**, 15, 989-99	1.3	37
157	Predictive Morphology Control of Hydrogen-Terminated Silicon Nanoparticles. *Journal of Physical Chemistry C*, **2014**, 118, 2580-2586	3.8	11
156	Shape dependence of the band gaps in luminescent silicon quantum dots. *Journal of Materials Chemistry C*, **2014**, 2, 9451-9456	7.1	17
155	Anisotropic adsorption and distribution of immobilized carboxyl on nanodiamond. *Nanoscale*, **2014**, 6, 14185-9	7.7	25
154	Molecular ionization and deprotonation energies as indicators of functional coating performance. *Journal of Materials Chemistry A*, **2014**, 2, 16660-16668	13	15
153	The impact of structural polydispersivity on the surface electrostatic potential of nanodiamond. *Nanoscale*, **2014**, 6, 1188-94	7.7	29
152	Optimal vacancy concentrations to maximize the NV yield in nanodiamonds. *Materials Horizons*, **2014**, 1, 286	14.4	9
151	Clarifying stability, probability and population in nanoparticle ensembles. *Nanoscale*, **2014**, 6, 9983-90	7.7	17

150	Size and shape dependent deprotonation potential and proton affinity of nanodiamond. *Nanotechnology*, **2014**, 25, 445702	3.4	16
149	Thermodynamic Control of Halogen-Terminated Silicon Nanoparticle Morphology. *Crystal Growth and Design*, **2014**, 14, 4468-4474	3.5	7
148	Contrasting Effects of Nanoparticle Binding on Protein Denaturation. *Journal of Physical Chemistry C*, **2014**, 118, 22069-22078	3.8	28
147	Towards chromate-free corrosion inhibitors: structure–property models for organic alternatives. *Green Chemistry*, **2014**, 16, 3349-3357	10	93
146	Activity of ZnO polar surfaces: an insight from surface energies. *Physical Chemistry Chemical Physics*, **2014**, 16, 22139-44	3.6	67
145	In silico veritas. *ACS Nano*, **2014**, 8, 6520-5	16.7	10
144	Size, Shape, Stability, and Color of Plasmonic Silver Nanoparticles. *Journal of Physical Chemistry C*, **2014**, 118, 9128-9136	3.8	117
143	Tuning the Electron Transfer Properties of Entire Nanodiamond Ensembles. *Journal of Physical Chemistry C*, **2014**, 118, 30209-30215	3.8	11
142	Diamond nanoparticles as a new platform for the sequestration of waste carbon. *Physical Chemistry Chemical Physics*, **2013**, 15, 9156-62	3.6	7
141	Modeling the Impact of Alkanethiol SAMs on the Morphology of Gold Nanocrystals. *Crystal Growth and Design*, **2013**, 13, 5433-5441	3.5	13
140	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
139	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
138	Can hematite nanoparticles be an environmental indicator?. *Energy and Environmental Science*, **2013**, 6, 561-569	35.4	24
137	Mapping the structural and optical properties of anisotropic gold nanoparticles. *Journal of Materials Chemistry C*, **2013**, 1, 3150	7.1	11
136	Modeling polydispersive ensembles of diamond nanoparticles. *Nanotechnology*, **2013**, 24, 085703	3.4	18
135	Naturally occurring iron oxide nanoparticles: morphology, surface chemistry and environmental stability. *Journal of Materials Chemistry A*, **2013**, 1, 27-42	13	170
134	Relative Stability of Graphene Nanoflakes Under Environmentally Relevant Conditions. *Journal of Physical Chemistry C*, **2013**, 117, 15375-15382	3.8	14
133	Technology: Sharing data in materials science. *Nature*, **2013**, 503, 463-4	50.4	8

132	Surface phase diagram and thermodynamic stability of functionalisation of nanodiamonds. *Journal of Materials Chemistry*, **2012**, 22, 16774		22
131	Modelling nanoscale cubic ZnS morphology and thermodynamic stability under sulphur-rich conditions. *CrystEngComm*, **2012**, 14, 7749	3.3	6
130	Nanodiamond for hydrogen storage: temperature-dependent hydrogenation and charge-induced dehydrogenation. *Nanoscale*, **2012**, 4, 1130-7	7.7	19
129	Ripple induced changes in the wavefunction of graphene: an example of a fundamental symmetry breaking. *Nanoscale*, **2012**, 4, 1167-70	7.7	16
128	High throughput theory and simulation of nanomaterials: exploring the stability and electronic properties of nanographene. *Journal of Materials Chemistry*, **2012**, 22, 18119		20
127	Surface phase diagram of hematite pseudocubes in hydrous environments. *Journal of Materials Chemistry*, **2012**, 22, 161-167		11
126	Modelling the role of size, edge structure and terminations on the electronic properties of trigonal graphene nanoflakes. *Nanotechnology*, **2012**, 23, 065707	3.4	25
125	Size- and shape-dependent phase transformations in wurtzite ZnS nanostructures. *Physical Chemistry Chemical Physics*, **2012**, 14, 9871-9	3.6	24
124	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
123	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
122	Modeling Nanomorphology in Noble Metal Particles: Thermodynamic Cartography **2012**, 269-303		1
121	Stability of Diamond at the Nanoscale **2012**, 3-52		1
120	Environmentally dependent stability of low-index hematite surfaces. *Journal of Colloid and Interface Science*, **2012**, 386, 315-24	9.3	19
119	Quantum mechanical properties of graphene nano-flakes and quantum dots. *Nanoscale*, **2012**, 4, 6761-7	7.7	30
118	Stability of Porous Platinum Nanoparticles: Combined In Situ TEM and Theoretical Study. *Journal of Physical Chemistry Letters*, **2012**, 3, 1106-10	6.4	12
117	Creation and luminescence of size-selected gold nanorods. *Nanoscale*, **2012**, 4, 5017-22	7.7	11
116	Charge-induced restructuring and decomposition of bucky-diamonds. *Journal of Materials Chemistry*, **2012**, 22, 13141		4
115	Interparticle Interactions and Self-Assembly of Functionalized Nanodiamonds. *Journal of Physical Chemistry Letters*, **2012**, 3, 896-901	6.4	35

114	Mapping the shape and phase of palladium nanocatalysts. *Catalysis Science and Technology*, **2012**, 2, 1485	5.5	18
113	Direct comparison of kinetic and thermodynamic influences on gold nanomorphology. *Accounts of Chemical Research*, **2012**, 45, 1688-97	24.3	59
112	Modelling of the reactivity and stability of carbon nanotubes under environmentally relevant conditions. *Physical Chemistry Chemical Physics*, **2012**, 14, 10080-93	3.6	13
111	Surface Area Limited Model for Predicting Anisotropic Coarsening of Faceted Nanoparticles. *Crystal Growth and Design*, **2011**, 11, 158-165	3.5	19
110	Mapping the photocatalytic activity or potential free radical toxicity of nanoscale titania. *Energy and Environmental Science*, **2011**, 4, 439-443	35.4	10
109	Modeling the thermostability of surface functionalisation by oxygen, hydroxyl, and water on nanodiamonds. *Nanoscale*, **2011**, 3, 2566-75	7.7	57
108	Confirmation of the electrostatic self-assembly of nanodiamonds. *Nanoscale*, **2011**, 3, 958-62	7.7	108
107	Proton transfer in the hydrogen-bonded chains of lepidocrocite: a computational study. *Physical Chemistry Chemical Physics*, **2011**, 13, 17864-9	3.6	7
106	Thermodynamic modelling of nanomorphologies of hematite and goethite. *Journal of Materials Chemistry*, **2011**, 21, 11566		95
105	Kinetic modelling of the shape-dependent evolution of faceted gold nanoparticles. *Journal of Materials Chemistry*, **2011**, 21, 12239		22
104	Stability of Nanodiamond Surfaces Exposed to N, NH, and NH2. *Journal of Physical Chemistry C*, **2011**, 115, 6218-6228	3.8	39
103	Atomistic simulation and measurement of pH dependent cancer therapeutic interactions with nanodiamond carrier. *Molecular Pharmaceutics*, **2011**, 8, 368-74	5.6	97
102	Useful equations for modeling the relative stability of common nanoparticle morphologies. *Computer Physics Communications*, **2011**, 182, 11-13	4.2	13
101	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
100	Morphology mapping of platinum catalysts over the entire nanoscale. *Catalysis Science and Technology*, **2011**, 1, 1440	5.5	24
99	A comparative density functional theory investigation of the mechanical and energetic properties of ZnS. *Molecular Simulation*, **2011**, 37, 321-333	2	7
98	Thermodynamic Cartography and Structure/Property Mapping of Commercial Platinum Catalysts. *ACS Catalysis*, **2011**, 1, 76-81	13.1	25
97	Modeling the iron oxides and oxyhydroxides for the prediction of environmentally sensitive phase transformations. *Physical Review B*, **2011**, 83,	3.3	58

96	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
95	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
94	One-to-one comparison of sunscreen efficacy, aesthetics and potential nanotoxicity. *Nature Nanotechnology*, **2010**, 5, 271-4	28.7	69
93	Resolving the structure of active sites on platinum catalytic nanoparticles. *Nano Letters*, **2010**, 10, 3073-6	11.5	94
92	Design of Nanodiamond Based Drug Delivery Patch for Cancer Therapeutics and Imaging Applications **2010**, 249-284		2
91	Safe, stable and effective nanotechnology: phase mapping of ZnS nanoparticles. *Journal of Materials Chemistry*, **2010**, 20, 4971		54
90	Observation and control of blinking nitrogen-vacancy centres in discrete nanodiamonds. *Nature Nanotechnology*, **2010**, 5, 345-9	28.7	354
89	Size- and shape-dependence of the graphene to graphane transformation in the absence of hydrogen. *Journal of Materials Chemistry*, **2010**, 20, 10459		28
88	Origin of nanomorphology: does a complete theory of nanoparticle evolution exist?. *Journal of Materials Chemistry*, **2010**, 20, 416-421		61
87	Morphological and phase stability of zinc blende, amorphous and mixed core-shell ZnS nanoparticles. *Nanoscale*, **2010**, 2, 2294-301	7.7	26
86	Modelling of nanoparticles: approaches to morphology and evolution. *Reports on Progress in Physics* , **2010**, 73, 086502	14.4	147
85	Transformation of graphene into graphane in the absence of hydrogen. *Carbon*, **2010**, 48, 981-986	10.4	25
84	Modeling the environmental stability of FeS2 nanorods, using lessons from biomineralization. *Nanotechnology*, **2009**, 20, 115702	3.4	6
83	Modelling the relative stability of carbon nanotubes exposed to environmental adsorbates and air. *Journal of Physics Condensed Matter*, **2009**, 21, 144205	1.8	2
82	Nanogold: a quantitative phase map. *ACS Nano*, **2009**, 3, 1431-6	16.7	197
81	Nanodiamond Photoemitters Based on Strong Narrow-Band Luminescence from Silicon-Vacancy Defects. *Advanced Materials*, **2009**, 21, 808-812	24	108
80	Partnerships for sustainable nanotechnology. *Materials Today*, **2009**, 12, 47	21.8	2
79	How can ab initio simulations address risks in nanotech?. *Nature Nanotechnology*, **2009**, 4, 332-5	28.7	48

78	Diamond standard in diagnostics: nanodiamond biolabels make their mark. *Analyst, The*, **2009**, 134, 1751-64	3.6	126
77	Thermodynamic stability and electronic structure of small carbon nitride nanotubes. *Journal of Physics Condensed Matter*, **2009**, 21, 144203	1.8	16
76	Morphological Stability of Pyrite FeS2 Nanocrystals in Water. *Journal of Physical Chemistry C*, **2009**, 113, 5376-5380	3.8	16
75	Shape-Dependent Confinement of the Nanodiamond Band Gap. *Crystal Growth and Design*, **2009**, 9, 4860-4863	3.5	36
74	Predicting the distribution and stability of photoactive defect centers in nanodiamond biomarkers. *Journal of Materials Chemistry*, **2009**, 19, 360-365		33
73	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
72	Computational strategies for predicting the potential risks associated with nanotechnology. *Nanoscale*, **2009**, 1, 89-95	7.7	24
71	Modelling nanoscale FeS2 formation in sulfur rich conditions. *Journal of Materials Chemistry*, **2009**, 19, 3389		34
70	An environmentally sensitive phase map of titania nanocrystals. *ACS Nano*, **2008**, 2, 2237-42	16.7	78
69	Ideality versus Reality: Emergence of the Chui Icosahedron. *Journal of Physical Chemistry C*, **2008**, 112, 14848-14852	3.8	10
68	Combining Theory and Experiment in Determining the Surface Chemistry of Nanocrystals. *Chemistry of Materials*, **2008**, 20, 5460-5463	9.6	30
67	Self-assembly in nanodiamond agglutinates. *Journal of Materials Chemistry*, **2008**, 18, 4038		139
66	Shape, Orientation, and Stability of Twinned Gold Nanorods. *Journal of Physical Chemistry C*, **2008**, 112, 1385-1390	3.8	15
65	Hybrid carbon nanotube/nanodiamond structures as electron emitters for cold cathodes. *Journal of Nanoscience and Nanotechnology*, **2008**, 8, 1989-93	1.3	10
64	Vacancy Induced Structural Changes in Diamond Nanoparticles. *Journal of Computational and Theoretical Nanoscience*, **2008**, 5, 2089-2095	0.3	19
63	Thermal stability of graphene edge structure and graphene nanoflakes. *Journal of Chemical Physics*, **2008**, 128, 094707	3.9	68
62	Modeling the preferred shape, orientation and aspect ratio of gold nanorods. *Journal of Materials Chemistry*, **2007**, 17, 3315		36
61	First Principles and Thermodynamic Modeling of CdS Surfaces and Nanorods. *Journal of Physical Chemistry C*, **2007**, 111, 18112-18117	3.8	40

60	Shape and Thermodynamic Stability of Pyrite FeS2Nanocrystals and Nanorods. *Journal of Physical Chemistry C*, **2007**, 111, 11742-11746	3.8	47
59	Crystallinity and surface electrostatics of diamond nanocrystals. *Journal of Materials Chemistry*, **2007**, 17, 4811		199
58	Can we predict the location of impurities in diamond nanoparticles?. *Diamond and Related Materials* , **2007**, 16, 2078-2082	3.5	35
57	Mapping the location and configuration of nitrogen in diamond nanoparticles. *Nanotechnology*, **2007**, 18, 025702	3.4	33
56	ZnO nanowires and nanobelts: Shape selection and thermodynamic modeling. *Applied Physics Letters*, **2007**, 90, 143116	3.4	69
55	Bonding and structure in BxNy nanotubes (x,y = 1,2). *Journal of Materials Chemistry*, **2007**, 17, 2892		11
54	Thermodynamic Modeling of Hydrogen Adsorption on Carbon Nanotubes During CVD Growth. *Chemical Vapor Deposition*, **2006**, 12, 388-394		2
53	Predicting the shape and structure of face-centered cubic gold nanocrystals smaller than 3 nm. *ChemPhysChem*, **2006**, 7, 1544-53	3.2	68
52	Modelling the formation of high aspect CdSe quantum wires: axial-growth versus oriented-attachment mechanisms. *Nanotechnology*, **2006**, 17, 5707-14	3.4	33
51	Modelling the effect of particle shape on the phase stability of ZrO2nanoparticles. *Nanotechnology*, **2006**, 17, 3039-3047	3.4	47
50	Using theory and modelling to investigate shape at the nanoscale. *Journal of Materials Chemistry*, **2006**, 16, 813-815		35
49	Theory and modeling of nanocarbon phase stability. *Diamond and Related Materials*, **2006**, 15, 285-291	3.5	31
48	Modeling the structure and electronic properties of TiO2 nanoparticles. *Physical Review B*, **2006**, 73,	3.3	52
47	Substitutional boron in nanodiamond, bucky-diamond, and nanocrystalline diamond grain boundaries. *Journal of Physical Chemistry B*, **2006**, 110, 19307-14	3.4	44
46	A thermodynamic model for the shape and stability of twinned nanostructures. *Journal of Physical Chemistry B*, **2006**, 110, 24498-504	3.4	97
45	Stability of Nanodiamond **2006**, 117-154		6
44	Carbon Family at the Nanoscale **2006**, 3-22		6
43	Nanohazards: knowledge is our first defence. *Nature Materials*, **2006**, 5, 245-8	27	76

42	Modelling the shape and orientation of ZnO nanobelts. *Chemical Physics Letters*, **2006**, 419, 313-316	2.5	20
41	First-principles modeling of dopants in C29 and C29H24 nanodiamonds. *Journal of Physical Chemistry B*, **2005**, 109, 11991-5	3.4	11
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