George Opletal

List of Publications by Year
in descending order

47 papers	1,215 citations	489802 18 h-index	425179 34 g-index
51 all docs	51 docs citations	51 times ranked	1658 citing authors

#	Article	IF	Citations
1	Simulating the fabrication of aluminium oxide tunnel junctions. Npj Quantum Information, 2021, 7, .	2.8	16
2	Extracting nanoscale structures from experimental and synthetic data with reverse Monte Carlo. Nano Futures, 2021, 5, 022502.	1.0	0
3	The pure and representative types of disordered platinum nanoparticles from machine learning. Nanotechnology, 2021, 32, 095404.	1.3	8
4	Study of amorphous boron carbide (a-BxC) materials using Molecular Dynamics (MD) and Hybrid Reverse Monte Carlo (HRMC). Journal of Non-Crystalline Solids, 2020, 530, 119783.	1.5	4
5	Classification of platinum nanoparticle catalysts using machine learning. Journal of Applied Physics, 2020, 128, .	1.1	24
6	Simulating facet-dependent aggregation and assembly of distributions of polyhedral nanoparticles. Nanoscale, 2020, 12, 19870-19879.	2.8	10
7	Selecting machine learning models for metallic nanoparticles. Nano Futures, 2020, 4, 035003.	1.0	22
8	Simulated nanoparticle assembly using protoparticles (SNAP). JPhys Materials, 2020, 3, 026001.	1.8	3
9	Dynamic self-assembly of detonation nanodiamond in water. Nanoscale, 2020, 12, 5363-5367.	2.8	34
10	Feature Engineering of Solidâ€State Crystalline Lattices for Machine Learning. Advanced Theory and Simulations, 2020, 3, 1900190.	1.3	3
11	Nanoinformatics, and the big challenges for the science of small things. Nanoscale, 2019, 11, 19190-19201.	2.8	59
12	Does Twinning Impact Structure/Property Relationships in Diamond Nanoparticles?. Journal of Physical Chemistry C, 2019, 123, 11207-11215.	1.5	9
13	Vacancy induced formation of nanoporous silicon, carbon and silicon carbide. Physical Chemistry Chemical Physics, 2019, 21, 6517-6524.	1.3	7
14	Predicting structure/property relationships in multi-dimensional nanoparticle data using t-distributed stochastic neighbour embedding and machine learning. Nanoscale, 2019, 11, 23165-23172.	2.8	24
15	PorosityPlus: characterisation of defective, nanoporous and amorphous materials. JPhys Materials, 2018, 1, 016002.	1.8	14
16	Correlating anisotropy and disorder with the surface structure of platinum nanoparticles. Nanoscale, 2018, 10, 20393-20404.	2.8	8
17	From Process to Properties: Correlating Synthesis Conditions and Structural Disorder of Platinum Nanocatalysts. Journal of Physical Chemistry C, 2018, 122, 28085-28093.	1.5	14
18	On reverse Monte Carlo constraints and model reproduction. Journal of Computational Chemistry, 2017, 38, 1547-1551.	1.5	10

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19	Predicting the role of seed morphology in the evolution of anisotropic nanocatalysts. Nanoscale, 2017, 9, 1502-1510.	2.8	10
20	Constructingab initiomodels of ultra-thin Alâ€“AlO_xâ€“Al barriers. Molecular Simulation, 2016, 42, 542-548.	0.9	12
21	Hybrid Reverse Monte Carlo and electron phase contrast image simulations of amorphous silicon with and without paracrystals. Molecular Simulation, 2016, 42, 522-530.	0.9	2
22	Dynamic evolution of specific catalytic sites on Pt nanoparticles. Catalysis Science and Technology, 2016, 6, 144-151.	2.1	23
23	Ab Initio Comparison of Bonding Environments and Threshold Behavior in Ge_xAs₁₀Se_{90â€“x} and Ge_xSb₁₀Se_{90â€“x} Glass Models. Journal of Physical Chemistry A, 2015, 119, 6421-6427.	1.1	5
24	Scalable and Fault-Tolerant Cloud Computations: Modelling and Implementation. , 2015, , .		7
25	Chiminey: Reliable Computing and Data Management Platform in the Cloud. , 2015, , .		14
26	Structural Modeling of Ge_{6.25}As_{32.5}Se_{61.25} Using a Combination of Reverse Monte Carlo and Ab Initio Molecular Dynamics. Journal of Physical Chemistry A, 2014, 118, 4790-4796.	1.1	8
27	HRMC_2.1: Hybrid Reverse Monte Carlo method with silicon, carbon, germanium and silicon carbide potentials. Computer Physics Communications, 2014, 185, 1854-1855.	3.0	15
28	Investigation of bonding within ab initio models of GeAsSe glasses. Chemical Physics Letters, 2013, 575, 97-100.	1.2	3
29	HRMC_2.0: Hybrid Reverse Monte Carlo method with silicon, carbon and germanium potentials. Computer Physics Communications, 2013, 184, 1946-1957.	3.0	27
30	Structural Modelling of Silicon Carbide-Derived Nanoporous Carbon by Hybrid Reverse Monte Carlo Simulation. Journal of Physical Chemistry C, 2013, 117, 14081-14094.	1.5	60
31	Bonding trends within ternary isocoordinate chalcogenide glasses GexAySe1âˆ’xâˆ’y. Physical Chemistry Chemical Physics, 2013, 15, 4582.	1.3	9
32	Study of the Initial Stage of Solid Electrolyte Interphase Formation upon Chemical Reaction of Lithium Metal and N-Methyl-N-Propyl-Pyrrolidinium-Bis(Fluorosulfonyl)Imide. Journal of Physical Chemistry C, 2012, 116, 19789-19797.	1.5	178
33	Crystallization in suspensions of hard spheres: a Monte Carlo and molecular dynamics simulation study. Journal of Physics Condensed Matter, 2011, 23, 194120.	0.7	23
34	Stability and Transformations of Heated Gold Nanorods. Journal of Physical Chemistry C, 2011, 115, 4375-4380.	1.5	29
35	HRMC_1.1: Hybrid Reverse Monte Carlo method with silicon and carbon potentials. Computer Physics Communications, 2011, 182, 542.	3.0	3
36	Precursor-Mediated Crystallization Process in Suspensions of Hard Spheres. Physical Review Letters, 2010, 105, 025701.	2.9	175

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37	Modeling the crystallization of gold nanoclustersâ€"the effect of the potential energy function. Journal of Physics Condensed Matter, 2009, 21, 144207.	0.7	5
38	A theoretical study of size and temperature dependent morphology transformations in gold nanoparticles. Chemical Physics Letters, 2009, 474, 115-118.	1.2	5
39	Elucidation of surface driven crystallization of icosahedral clusters. Chemical Physics Letters, 2009, 482, 281-286.	1.2	8
40	HRMC: Hybrid Reverse Monte Carlo method with silicon and carbon potentials. Computer Physics Communications, 2008, 178, 777-787.	3.0	30
41	Ideality versus Reality: Emergence of the Chui Icosahedron. Journal of Physical Chemistry C, 2008, 112, 14848-14852.	1.5	12
42	Modeling of structure and porosity in amorphous silicon systems using Monte Carlo methods. Journal of Chemical Physics, 2007, 126, 214705.	1.2	19
43	The structure of disordered carbon solids studied using a hybrid reverse Monte Carlo algorithm. Journal of Physics Condensed Matter, 2005, 17, 2605-2616.	0.7	36
44	Microstructure of an industrial char by diffraction techniques and Reverse Monte Carlo modelling. Carbon, 2004, 42, 2457-2469.	5.4	55
45	Structural analysis of carbonaceous solids using an adapted reverse Monte Carlo algorithm. Carbon, 2003, 41, 2403-2411.	5.4	55
46	Hybrid approach for generating realistic amorphous carbon structure using metropolis and reverse Monte Carlo. Molecular Simulation, 2002, 28, 927-938.	0.9	116
47	Simulating Facetâ€Dependent Aggregation and Assembly of Mixtures of Polyhedral Nanoparticles. Advanced Theory and Simulations, 0, , 2100279.	1.3	2