Duncan John Mowbray

List of Publications by Year
in descending order

84	2,729	172443	182417
papers	citations	29 h-index	51 g-index

85	85	85	3846
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Impact of the Solvent Composition on the Structural and Mechanical Properties of Customizable Electrospun Poly(Vinylpyrrolidone) Fiber Mats. Physical Chemistry Chemical Physics, 2021, 23, 22923-22935.	2.8	4
2	Unveiling Adatoms in On-Surface Reactions: Combining Scanning Probe Microscopy with vanâ€™t Hoff Plots. Journal of Physical Chemistry C, 2021, 125, 9847-9854.	3.1	8
3	Reassessing the Adsorption Behavior and on-Surface Reactivity of a Brominated Porphyrin on Cu(111). Journal of Physical Chemistry C, 2021, 125, 17164-17173.	3.1	9
4	Ab initio study of electromagnetic modes in two-dimensional semiconductors: Application to doped phosphorene. Physical Review B, 2021, 104, .	3.2	12
5	Theoretical study of electronic properties and chemical stability of cubic phase zirconia nanowires. Physica Scripta, 2021, 96, 125879.	2.5	1
6	Understanding the Electron-Doping Mechanism in Potassium-Intercalated Single-Walled Carbon Nanotubes. Journal of the American Chemical Society, 2020, 142, 2327-2337.	13.7	16
7	Conductivity models for electron energy loss spectroscopy of graphene in a scanning transmission electron microscope with high energy resolution. Ultramicroscopy, 2020, 214, 113012.	1.9	6
8	Supramolecular Ordering and Reactions of a Chlorophenyl Porphyrin on Ag(111). Journal of Physical Chemistry C, 2020, 124, 14220-14228.	3.1	9
9	LCAO-TDDFT-k- Ï‰ : spectroscopy in the optical limit. Journal of Physics Condensed Matter, 2020, 32, 415901.	1.8	3
10	Optical excitations of chlorophyll a and b monomers and dimers. Journal of Chemical Physics, 2019, 151, 174102.	3.0	9
11	Tailoring a Moleculeâ€™s Optical Absorbance Using Surface Plasmonics. Journal of Physical Chemistry C, 2019, 123, 26498-26508.	3.1	4
12	Tailoring Organicâ€“Organic Poly(vinylpyrrolidone) Microparticles and Fibers with Multiwalled Carbon Nanotubes for Reinforced Composites. ACS Applied Nano Materials, 2019, 2, 4302-4312.	5.0	17
13	Roles of Precursor Conformation and Adatoms in Ullmann Coupling: An Inverted Porphyrin on Cu(111). Chemistry of Materials, 2019, 31, 3009-3017.	6.7	22
14	An Archaeometric Characterization of Ecuadorian Pottery. Scientific Reports, 2019, 9, 2642.	3.3	3
15	Optical absorption and energy loss spectroscopy of single-walled carbon nanotubes. Physical Review B, 2019, 100, .	3.2	7
16	Density functional theory calculations of the radial breathing mode in graphene quantum dots. Journal of Nanophotonics, 2019, 13, 1.	1.0	2
17	Modelling relativistic effects in momentum-resolved electron energy loss spectroscopy of graphene. Radiation Effects and Defects in Solids, 2018, 173, 8-21.	1.2	5
18	Optical Absorption Spectra and Excitons of Dye-Substrate Interfaces: Catechol on TiO₂(110). Journal of Chemical Theory and Computation, 2016, 12, 2843-2852.	5.3	31

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19	Disentangling Vacancy Oxidation on Metallicity-Sorted Carbon Nanotubes. Journal of Physical Chemistry C, 2016, 120, 18316-18322.	3.1	8
20	Theoretical Insight into the Internal Quantum Efficiencies of Polymer/C60 and Polymer/SWNT Photovoltaic Devices. Journal of Physical Chemistry C, 2016, 120, 6336-6343.	3.1	2
21	Photoinduced Absorption within Single-Walled Carbon Nanotube Systems. Journal of Physical Chemistry C, 2016, 120, 1926-1935.	3.1	12
22	Quasiparticle Interfacial Level Alignment of Highly Hybridized Frontier Levels: H₂O on TiO₂(110). Journal of Chemical Theory and Computation, 2015, 11, 239-251.	5.3	28
23	Using G₀W₀ Level Alignment to Identify Catecholâ€™s Structure on TiO₂(110). Journal of Physical Chemistry C, 2015, 119, 19634-19641.	3.1	13
24	Quantum-ionic features in the absorption spectra of homonuclear diatomic molecules. Physical Review A, 2015, 91, .	2.5	1
25	Comparing Quasiparticle H₂O Level Alignment on Anatase and Rutile TiO₂. ACS Catalysis, 2015, 5, 4242-4254.	11.2	50
26	Calculation of the graphene C<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mi>s</mml:mi></mml:mrow></mml:n level binding energy. Physical Review B, 2015, 91, .	3.2	36
27	Theoretical electron energy loss spectroscopy of isolated graphene. Physica Status Solidi (B): Basic Research, 2014, 251, 2509-2514.	1.5	24
28	Gas Sensing and Thermal Transport Through Carbon-Nanotube-Based Nanodevices. Challenges and Advances in Computational Chemistry and Physics, 2014, , 99-136.	0.6	1
29	Modelling the effect of nuclear motion on the attosecond time-resolved photoelectron spectra of ethylene. Journal of Physics B: Atomic, Molecular and Optical Physics, 2014, 47, 124018.	1.5	11
30	Coverage dependence of the level alignment for methanol on TiO2(110). Computational and Theoretical Chemistry, 2014, 1040-1041, 259-265.	2.5	13
31	Photoinduced Câ€“C Reactions on Insulators toward Photolithography of Graphene Nanoarchitectures. Journal of the American Chemical Society, 2014, 136, 4651-4658.	13.7	45
32	Quasiparticle Level Alignment for Photocatalytic Interfaces. Journal of Chemical Theory and Computation, 2014, 10, 2103-2113.	5.3	60
33	Using surface plasmonics to turn on fullerene's dark excitons. Physical Review B, 2014, 89, .	3.2	12
34	Revealing the Adsorption Mechanisms of Nitroxides on Ultrapure, Metallicity-Sorted Carbon Nanotubes. ACS Nano, 2014, 8, 1375-1383.	14.6	31
35	Time-dependent density-functional theory of strong-field ionization of atoms by soft x rays. Physical Review A, 2014, 90, .	2.5	29
36	PFOâ€“BPy solubilizers for SWNTs: Modelling of polymers from oligomers. Physica Status Solidi (B): Basic Research, 2014, 251, 2407-2412.	1.5	6

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37	Level Alignment of a Prototypical Photocatalytic System: Methanol on TiO₂(110). Journal of the American Chemical Society, 2013, 135, 11429-11432.	13.7	68
38	Understanding Energy-Level Alignment in Donorâ€“Acceptor/Metal Interfaces from Core-Level Shifts. ACS Nano, 2013, 7, 6914-6920.	14.6	78
39	Gold and Methane: A Noble Combination for Delicate Oxidation. Journal of Physical Chemistry Letters, 2013, 4, 3006-3012.	4.6	28
40	Direct Imaging of Covalent Bond Structure in Single-Molecule Chemical Reactions. Science, 2013, 340, 1434-1437.	12.6	513
41	Quasiparticle spectra and excitons of organic molecules deposited on substrates:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mml:msub></mml:mrow></mml:math> approach applied to benzene on graphene and metallic substrates. Physical Review B, 2013, 88, .	3.2	19
42	Plasmon excitation in single wall carbon nanotubes by penetrating charged particles. Journal of Physics: Conference Series, 2012, 388, 132025.	0.4	0
43	Anomalous insulator-metal transition in boron nitride-graphene hybrid atomic layers. Physical Review B, 2012, 86, .	3.2	42
44	TDDFT study of time-dependent and static screening in graphene. Physical Review B, 2012, 86, .	3.2	29
45	Understanding Charge Transfer in Donorâ€“Acceptor/Metal Systems: A Combined Theoretical and Experimental Study. Journal of Physical Chemistry C, 2012, 116, 17991-18001.	3.1	37
46	Channeling of charge carrier plasmons in carbon nanotubes. Physical Review B, 2012, 85, .	3.2	12
47	Supramolecular Environment-Dependent Electronic Properties of Metalâ€“Organic Interfaces.. Journal of Physical Chemistry C, 2012, 116, 4780-4785.	3.1	25
48	Scanning Tunneling Microscopy Evidence for the Dissociation of Carbon Monoxide on Ruthenium Steps. Journal of Physical Chemistry C, 2012, 116, 14350-14359.	3.1	30
49	Solid-State Reactions in Binary Molecular Assemblies of F16CuPc and Pentacene. ACS Nano, 2011, 5, 581-589.	14.6	45
50	Computing C1<I>s</I> X-ray Absorption for Single-Walled Carbon Nanotubes with Distinct Electronic Type. Materials Express, 2011, 1, 225-230.	0.5	8
51	Trends in Metal Oxide Stability for Nanorods, Nanotubes, and Surfaces. Journal of Physical Chemistry C, 2011, 115, 2244-2252.	3.1	52
52	A Resonant Photoemission Insight to the Electronic Structure of Gd Nanowires Templated in the Hollow Core of SWCNTs. Materials Express, 2011, 1, 30-35.	0.5	20
53	Tailoring Electronic and Optical Properties of TiO₂: Nanostructuring, Doping and Molecular-Oxide Interactions. , 2011, , 301-329.		2
54	Tuning MgB<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>(0001) surface states through surface termination. Physical Review B, 2011, 84, .	3.2	6

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55	Self Blocking of CO Dissociation on a Stepped Ruthenium Surface. Topics in Catalysis, 2010, 53, 357-364.	2.8	44
56	Designing multifunctional chemical sensors using Ni and Cu doped carbon nanotubes. Physica Status Solidi (B): Basic Research, 2010, 247, 2678-2682.	1.5	8
57	A combined photoemission and ab initio study of the electronic structure of (6,4)/(6,5) enriched single wall carbon nanotubes. Physica Status Solidi (B): Basic Research, 2010, 247, 2875-2879.	1.5	3
58	The donut and dynamic polarization effects in proton channeling through carbon nanotubes. New Journal of Physics, 2010, 12, 043021.	2.9	20
59	Modeling nanoscale gas sensors under realistic conditions: Computational screening of metal-doped carbon nanotubes. Physical Review B, 2010, 81, .	3.2	37
60	Publisher's Note: Plasmon excitations on a single-wall carbon nanotube by external charges: Two-dimensional two-fluid hydrodynamic model [Phys. Rev. B82, 035405 (2010)]. Physical Review B, 2010, 82, .	3.2	1
61	Plasmon excitations on a single-wall carbon nanotube by external charges: Two-dimensional two-fluid hydrodynamic model. Physical Review B, 2010, 82, .	3.2	47
62	Combined experimental andab initiostudy of the electronic structure of narrow-diameter single-wall carbon nanotubes with predominant (6,4),(6,5) chirality. Physical Review B, 2010, 82, .	3.2	19
63	Trends in CO Oxidation Rates for Metal Nanoparticles and Close-Packed, Stepped, and Kinked Surfaces. Journal of Physical Chemistry C, 2009, 113, 10548-10553.	3.1	244
64	Density functional theory based screening of ternary alkali-transition metal borohydrides: A computational material design project. Journal of Chemical Physics, 2009, 131, 014101.	3.0	77
65	Influence ofO2andN2on the conductivity of carbon nanotube networks. Physical Review B, 2009, 79, .	3.2	55
66	Stability and Electronic Properties of TiO₂ Nanostructures With and Without B and N Doping. Journal of Physical Chemistry C, 2009, 113, 12301-12308.	3.1	102
67	Quantization of plasmon excitation in carbon nanotubes: Two-dimensional two-fluids hydrodynamic model. Journal of Physics: Conference Series, 2009, 194, 132008.	0.4	0
68	Oxidation of CO and H2 by O2 and N2O on Au/TiO2 catalysts in microreactors. Journal of Catalysis, 2008, 260, 86-92.	6.2	29
69	Dynamic polarization effects on the angular distributions of protons channeled through carbon nanotubes in dielectric media. Physical Review A, 2008, 77, .	2.5	23
70	Influence of functional groups on charge transport in molecular junctions. Journal of Chemical Physics, 2008, 128, 111103.	3.0	114
71	Channeling of protons through carbon nanotubes embedded in dielectric media. Journal of Physics Condensed Matter, 2008, 20, 474212.	1.8	12
72	Channeling of protons through carbon nanotubes. Journal of Physics: Conference Series, 2008, 133, 012015.	0.4	8

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73	Comparative study of anchoring groups for molecular electronics: structure and conductance of Auâ€“Sâ€“Au and Auâ€“NH2â€“Au junctions. Journal of Physics Condensed Matter, 2008, 20, 374101.	1.8	34
74	Channelling of dipolar molecules through carbon nanotubes. Nanotechnology, 2007, 18, 424034.	2.6	4
75	Stopping power for ion channeling through carbon nanotubes. Radiation Effects and Defects in Solids, 2007, 162, 523-530.	1.2	1
76	Influence of the dynamic polarization effect on the angular distributions of protons channeled in double-wall carbon nanotubes. Nuclear Instruments & Methods in Physics Research B, 2007, 256, 131-136.	1.4	11
77	Dynamic interactions of ions with carbon nanotubes in water. Nuclear Instruments & Methods in Physics Research B, 2007, 256, 167-171.	1.4	3
78	Dynamic interactions of fast ions with multiwalled carbon nanotubes. Radiation Physics and Chemistry, 2007, 76, 524-528.	2.8	14
79	Influence of the dynamical image potential on the rainbows in ion channeling through short carbon nanotubes. Physical Review A, 2006, 73, .	2.5	53
80	Ion interactions with carbon nanotubes in dielectric media. Physical Review B, 2006, 74, .	3.2	54
81	HYDRODYNAMIC MODELING OF FAST ION INTERACTIONS WITH CARBON NANOTUBES. , 2006, , 177-178.		0
82	Dynamic interactions of fast ions with carbon nanotubes. Nuclear Instruments & Methods in Physics Research B, 2005, 230, 142-147.	1.4	28
83	Wake effect in interactions of fast ions with carbon nanotubes. Physics Letters, Section A: General, Atomic and Solid State Physics, 2004, 329, 94-99.	2.1	33
84	Interactions of fast ions with carbon nanotubes:â€ƒTwo-fluid model. Physical Review B, 2004, 70, .	3.2	83