

# Neil D. Drummond

## List of Publications by Year in descending order

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53  
papers

5,595  
citations

159358

30  
h-index

161609

54  
g-index

55  
all docs

55  
docs citations

55  
times ranked

6284  
citing authors

#	ARTICLE	IF	CITATIONS
1	Electrically tunable band gap in silicene. <i>Physical Review B</i> , 2012, 85, .	1.1	997
2	$k \cdot p$ theory for two-dimensional transition metal dichalcogenide semiconductors. <i>2D Materials</i> , 2015, 2, 022001.	2.0	676
3	Monolayer MoS <sub>2</sub> : Trigonal warping, the $\Gamma$ -valley, and spin-orbit coupling effects. <i>Physical Review B</i> , 2013, 88, .	1.1	357
4	High-Sensitivity Photodetectors Based on Multilayer GaTe Flakes. <i>ACS Nano</i> , 2014, 8, 752-760.	7.3	319
5	Continuum variational and diffusion quantum Monte Carlo calculations. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 023201.	0.7	306
6	Electrons and phonons in single layers of hexagonal indium chalcogenides from $ab$ initio calculations. <i>Physical Review B</i> , 2014, 89, .	1.1	281
7	Spin-Orbit Coupling, Quantum Dots, and Qubits in Monolayer Transition Metal Dichalcogenides. <i>Physical Review X</i> , 2014, 4, .	2.8	222
8	Inhomogeneous backflow transformations in quantum Monte Carlo calculations. <i>Physical Review E</i> , 2006, 74, 066701.	0.8	204
9	Band structure and optical transitions in atomic layers of hexagonal gallium chalcogenides. <i>Physical Review B</i> , 2013, 87, .	1.1	181
10	Finite-size errors in continuum quantum Monte Carlo calculations. <i>Physical Review B</i> , 2008, 78, .	1.1	173
11	Quantum Monte Carlo Calculation of the Binding Energy of Bilayer Graphene. <i>Physical Review Letters</i> , 2015, 115, 115501.	2.9	166
12	Electron Emission from Diamondoids: A Diffusion Quantum Monte Carlo Study. <i>Physical Review Letters</i> , 2005, 95, 096801.	2.9	154
13	Anharmonic vibrational properties in periodic systems: energy, electron-phonon coupling, and stress. <i>Physical Review B</i> , 2013, 87, .	1.1	151
14	Phase Diagram of the Low-Density Two-Dimensional Homogeneous Electron Gas. <i>Physical Review Letters</i> , 2009, 102, 126402.	2.9	96
15	Three-Particle Complexes in Two-Dimensional Semiconductors. <i>Physical Review Letters</i> , 2015, 114, 107401.	2.9	88
16	Quantum Monte Carlo study of the phase diagram of solid molecular hydrogen at extreme pressures. <i>Nature Communications</i> , 2015, 6, 7794.	5.8	84
17	Variational and diffusion quantum Monte Carlo calculations with the CASINO code. <i>Journal of Chemical Physics</i> , 2020, 152, 154106.	1.2	84
18	Quantum Monte Carlo study of the three-dimensional spin-polarized homogeneous electron gas. <i>Physical Review B</i> , 2013, 88, .	1.1	79

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19	Scheme for adding electron-nucleus cusps to Gaussian orbitals. <i>Journal of Chemical Physics</i> , 2005, 122, 224322.	1.2	74
20	Quantum Monte Carlo Study of a Positron in an Electron Gas. <i>Physical Review Letters</i> , 2011, 107, 207402.	2.9	68
21	Electron-Phonon Coupling and the Metallization of Solid Helium at Terapascal Pressures. <i>Physical Review Letters</i> , 2014, 112, 055504.	2.9	64
22	All-electron quantum Monte Carlo calculations for the noble gas atoms He to Xe. <i>Physical Review E</i> , 2005, 71, 066704.	0.8	56
23	Exciton-exciton interaction and biexciton formation in bilayer systems. <i>Physical Review B</i> , 2009, 79, .	1.1	40
24	Framework for constructing generic Jastrow correlation factors. <i>Physical Review E</i> , 2012, 86, 036703.	0.8	40
25	Quantum Monte Carlo, density functional theory, and pair potential studies of solid neon. <i>Physical Review B</i> , 2006, 73, .	1.1	36
26	van der Waals Interactions between Thin Metallic Wires and Layers. <i>Physical Review Letters</i> , 2007, 99, 166401.	2.9	36
27	Quantum Monte Carlo studies of covalent and metallic clusters: Accuracy of density functional approximations. <i>Physical Review B</i> , 2009, 79, .	1.1	36
28	Quantum Monte Carlo study of the Ne atom and the Ne <sup>+</sup> ion. <i>Journal of Chemical Physics</i> , 2006, 124, 224104.	1.2	35
29	Ground-state properties of the one-dimensional electron liquid. <i>Physical Review B</i> , 2011, 83, .	1.1	35
30	Optoelectronic properties of atomically thin ReSSe with weak interlayer coupling. <i>Nanoscale</i> , 2016, 8, 5826-5834.	2.8	32
31	Quasiparticle and excitonic gaps of one-dimensional carbon chains. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 14810-14821.	1.3	31
32	Diamond to $\beta$ -tin phase transition in Si within diffusion quantum Monte Carlo. <i>Physical Review B</i> , 2010, 82, .	1.1	30
33	The physics of single-side fluorination of graphene: DFT and DFT+U studies. <i>Carbon</i> , 2019, 144, 615-627.	5.4	30
34	Quantum Monte Carlo study of the ground state of the two-dimensional Fermi fluid. <i>Physical Review B</i> , 2009, 79, .	1.1	29
35	Bulk and surface energetics of crystalline lithium hydride: Benchmarks from quantum Monte Carlo and quantum chemistry. <i>Physical Review B</i> , 2010, 82, .	1.1	27
36	Quantum Monte Carlo calculations of the dissociation energies of three-electron hemibonded radical cationic dimers. <i>Journal of Chemical Physics</i> , 2006, 124, 024318.	1.2	26

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37	Comparison of quantum Monte Carlo with time-dependent and static density-functional theory calculations of diamondoid excitation energies and Stokes shifts. <i>Physical Review B</i> , 2011, 84, .	1.1	24
38	Anomalous nonadditive dispersion interactions in systems of three one-dimensional wires. <i>Physical Review B</i> , 2014, 89, .	1.1	23
39	Quantum Monte Carlo calculation of the energy band and quasiparticle effective mass of the two-dimensional Fermi fluid. <i>Physical Review B</i> , 2009, 80, .	1.1	22
40	Diamondoids display their potential. <i>Nature Nanotechnology</i> , 2007, 2, 462-463.	15.6	16
41	Quantum Monte Carlo calculation of the zero-temperature phase diagram of the two-component fermionic hard-core gas in two dimensions. <i>Physical Review B</i> , 2011, 83, .	1.1	16
42	First-principles method for impurities in quantum fluids: Positron in an electron gas. <i>Physical Review B</i> , 2010, 82, .	1.1	15
43	Diffusion quantum Monte Carlo calculation of the quasiparticle effective mass of the two-dimensional homogeneous electron gas. <i>Physical Review B</i> , 2013, 87, .	1.1	15
44	Performance of an ab initio equation of state for magnesium oxide. <i>Journal of Physics Condensed Matter</i> , 2004, 16, 5435-5442.	0.7	14
45	Trion formation in a two-dimensional hole-doped electron gas. <i>Physical Review B</i> , 2016, 94, .	1.1	14
46	Coulomb finite-size effects in quasi-two-dimensional systems. <i>Journal of Physics Condensed Matter</i> , 2004, 16, 891-902.	0.7	13
47	Quasiparticle Effective Mass of the Three-Dimensional Fermi Liquid by Quantum Monte Carlo. <i>Physical Review Letters</i> , 2021, 127, 086401.	2.9	12
48	Importance of high-angular-momentum channels in pseudopotentials for quantum Monte Carlo. <i>Physical Review B</i> , 2014, 90, .	1.1	8
49	A Variational Monte Carlo Study of Positronic Compounds Using Inhomogeneous Backflow Transformations. <i>Chemistry Letters</i> , 2010, 39, 1136-1137.	0.7	7
50	Quantum Monte Carlo calculation of the Fermi liquid parameters of the two-dimensional homogeneous electron gas. <i>Physical Review B</i> , 2013, 88, .	1.1	7
51	Structures of bulk hexagonal post transition metal chalcogenides from dispersion-corrected density functional theory. <i>Physical Review B</i> , 2021, 103, .	1.1	6
52	Ground-state properties of electron-electron biwire systems. <i>Physical Review B</i> , 2021, 104, .	1.1	5
53	Electron correlation and confinement effects in quasi-one-dimensional quantum wires at high density. <i>Physical Review B</i> , 2022, 105, .	1.1	3