Neil D. Drummond

List of Publications by Year
in descending order

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	Electron correlation and confinement effects in quasi-one-dimensional quantum wires at high density. Physical Review B, 2022, 105, .	1.1	3
2	Structures of bulk hexagonal post transition metal chalcogenides from dispersion-corrected density functional theory. Physical Review B, 2021, 103, .	1.1	6
3	Ground-state properties of electron-electron biwire systems. Physical Review B, 2021, 104, .	1.1	5
4	Quasiparticle Effective Mass of the Three-Dimensional Fermi Liquid by Quantum MonteÂCarlo. Physical Review Letters, 2021, 127, 086401.	2.9	12
5	Variational and diffusion quantum Monte Carlo calculations with the CASINO code. Journal of Chemical Physics, 2020, 152, 154106.	1.2	84
6	The physics of single-side fluorination of graphene: DFT and DFTÂ+ U studies. Carbon, 2019, 144, 615-627.	5.4	30
7	Trion formation in a two-dimensional hole-doped electron gas. Physical Review B, 2016, 94, .	1.1	14
8	Quasiparticle and excitonic gaps of one-dimensional carbon chains. Physical Chemistry Chemical Physics, 2016, 18, 14810-14821.	1.3	31
9	Optoelectronic properties of atomically thin ReSSe with weak interlayer coupling. Nanoscale, 2016, 8, 5826-5834.	2.8	32
10	Quantum MonteÂCarlo Calculation of the Binding Energy of Bilayer Graphene. Physical Review Letters, 2015, 115, 115501.	2.9	166
11	Three-Particle Complexes in Two-Dimensional Semiconductors. Physical Review Letters, 2015, 114, 107401.	2.9	88
12	k Â· p theory for two-dimensional transition metal dichalcogenide semiconductors. 2D Materials, 2015, 2, 022001.	2.0	676
13	Quantum Monte Carlo study of the phase diagram of solid molecular hydrogen at extreme pressures. Nature Communications, 2015, 6, 7794.	5.8	84
14	Importance of high-angular-momentum channels in pseudopotentials for quantum Monte Carlo. Physical Review B, 2014, 90, .	1.1	8
15	Electron-Phonon Coupling and the Metallization of Solid Helium at Terapascal Pressures. Physical Review Letters, 2014, 112, 055504.	2.9	64
16	Spin-Orbit Coupling, Quantum Dots, and Qubits in Monolayer Transition Metal Dichalcogenides. Physical Review X, 2014, 4, .	2.8	222
17	Anomalous nonadditive dispersion interactions in systems of three one-dimensional wires. Physical Review B, 2014, 89, .	1.1	23
18	High-Sensitivity Photodetectors Based on Multilayer GaTe Flakes. ACS Nano, 2014, 8, 752-760.	7.3	319

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19	Electrons and phonons in single layers of hexagonal indium chalcogenides fromab initiocalculations. Physical Review B, 2014, 89, .	1.1	281
20	Anharmonic vibrational properties in periodic systems: energy, electron-phonon coupling, and stress. Physical Review B, 2013, 87, .	1.1	151
21	Quantum Monte Carlo study of the three-dimensional spin-polarized homogeneous electron gas. Physical Review B, 2013, 88, .	1.1	79
22	Monolayer MoS<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>: Trigonal warping, the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î“</mml:mi></mml:math>valley, and spin-orbit coupling effects. Physical Review B, 2013, 88, .	1.1	357
23	Diffusion quantum Monte Carlo calculation of the quasiparticle effective mass of the two-dimensional homogeneous electron gas. Physical Review B, 2013, 87, .	1.1	15
24	Band structure and optical transitions in atomic layers of hexagonal gallium chalcogenides. Physical Review B, 2013, 87, .	1.1	181
25	Quantum Monte Carlo calculation of the Fermi liquid parameters of the two-dimensional homogeneous electron gas. Physical Review B, 2013, 88, .	1.1	7
26	Electrically tunable band gap in silicene. Physical Review B, 2012, 85, .	1.1	997
27	Framework for constructing generic Jastrow correlation factors. Physical Review E, 2012, 86, 036703.	0.8	40
28	Comparison of quantum Monte Carlo with time-dependent and static density-functional theory calculations of diamondoid excitation energies and Stokes shifts. Physical Review B, 2011, 84, .	1.1	24
29	Quantum MonteÂCarlo Study of a Positron in an Electron Gas. Physical Review Letters, 2011, 107, 207402.	2.9	68
30	Quantum Monte Carlo calculation of the zero-temperature phase diagram of the two-component fermionic hard-core gas in two dimensions. Physical Review B, 2011, 83, .	1.1	16
31	Ground-state properties of the one-dimensional electron liquid. Physical Review B, 2011, 83, .	1.1	35
32	A Variational Monte Carlo Study of Positronic Compounds Using Inhomogeneous Backflow Transformations. Chemistry Letters, 2010, 39, 1136-1137.	0.7	7
33	Continuum variational and diffusion quantum Monte Carlo calculations. Journal of Physics Condensed Matter, 2010, 22, 023201.	0.7	306
34	First-principles method for impurities in quantum fluids: Positron in an electron gas. Physical Review B, 2010, 82, .	1.1	15
35	Diamond toÎ²-tin phase transition in Si within diffusion quantum Monte Carlo. Physical Review B, 2010, 82, .	1.1	30
36	Bulk and surface energetics of crystalline lithium hydride: Benchmarks from quantum Monte Carlo and quantum chemistry. Physical Review B, 2010, 82, .	1.1	27

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37	Exciton-exciton interaction and biexciton formation in bilayer systems. Physical Review B, 2009, 79, .	1.1	40
38	Quantum Monte Carlo studies of covalent and metallic clusters: Accuracy of density functional approximations. Physical Review B, 2009, 79, .	1.1	36
39	Quantum Monte Carlo calculation of the energy band and quasiparticle effective mass of the two-dimensional Fermi fluid. Physical Review B, 2009, 80, .	1.1	22
40	Quantum Monte Carlo study of the ground state of the two-dimensional Fermi fluid. Physical Review B, 2009, 79, .	1.1	29
41	Phase Diagram of the Low-Density Two-Dimensional Homogeneous Electron Gas. Physical Review Letters, 2009, 102, 126402.	2.9	96
42	Finite-size errors in continuum quantum Monte Carlo calculations. Physical Review B, 2008, 78, .	1.1	173
43	van der Waals Interactions between Thin Metallic Wires and Layers. Physical Review Letters, 2007, 99, 166401.	2.9	36
44	Diamondoids display their potential. Nature Nanotechnology, 2007, 2, 462-463.	15.6	16
45	Quantum Monte Carlo calculations of the dissociation energies of three-electron hemibonded radical cationic dimers. Journal of Chemical Physics, 2006, 124, 024318.	1.2	26
46	Quantum Monte Carlo, density functional theory, and pair potential studies of solid neon. Physical Review B, 2006, 73, .	1.1	36
47	Inhomogeneous backflow transformations in quantum Monte Carlo calculations. Physical Review E, 2006, 74, 066701.	0.8	204
48	Quantum Monte Carlo study of the Ne atom and the Ne+ ion. Journal of Chemical Physics, 2006, 124, 224104.	1.2	35
49	All-electron quantum Monte Carlo calculations for the noble gas atoms He to Xe. Physical Review E, 2005, 71, 066704.	0.8	56
50	Scheme for adding electronâ€“nucleus cusps to Gaussian orbitals. Journal of Chemical Physics, 2005, 122, 224322.	1.2	74
51	Electron Emission from Diamondoids: A Diffusion Quantum Monte Carlo Study. Physical Review Letters, 2005, 95, 096801.	2.9	154
52	Coulomb finite-size effects in quasi-two-dimensional systems. Journal of Physics Condensed Matter, 2004, 16, 891-902.	0.7	13
53	Performance of an ab initio equation of state for magnesium oxide. Journal of Physics Condensed Matter, 2004, 16, 5435-5442.	0.7	14