Nikitas I Gidopoulos

List of Publications by Year
in descending order

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50	674	516710	580821
papers	citations	16	25
		h-index	g-index

50	50	50	503
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Electronic non-adiabatic states: towards a density functional theory beyond the Bornâ€“Oppenheimer approximation. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130059.	3.4	80
2	Breakdown of the Born-Oppenheimer description explains neutron Compton-scattering anomaly. Physical Review B, 2005, 71, .	3.2	49
3	Hartree-Fock equations determining the optimum set of spin orbitals for the expansion of excited states. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1994, 69, 1067-1074.	0.6	40
4	Constraining density functional approximations to yield self-interaction free potentials. Journal of Chemical Physics, 2012, 136, 224109.	3.0	36
5	Kohn-Sham equations for multicomponent systems: The exchange and correlation energy functional. Physical Review B, 1998, 57, 2146-2152.	3.2	35
6	Calculation of electronic excited states of molecules using the Helmholtz free-energy minimum principle. Physical Review A, 2013, 87, .	2.5	35
7	Born effective charge reversal and metallic threshold state at a band insulator-Mott insulator transition. European Physical Journal B, 2000, 14, 217-226.	1.5	32
8	Local reduced-density-matrix-functional theory: Incorporating static correlation effects in Kohn-Sham equations. Physical Review A, 2014, 90, .	2.5	32
9	Nonanalyticity of the optimized effective potential with finite basis sets. Physical Review A, 2012, 85, .	2.5	26
10	Potential in spin-density-functional theory of noncollinear magnetism determined by the many-electron ground state. Physical Review B, 2007, 75, .	3.2	25
11	Ensemble-Hartreeâ€“Fock scheme for excited states. The optimized effective potential method. Physica B: Condensed Matter, 2002, 318, 328-332.	2.7	24
12	Parametric representation of open quantum systems and cross-over from quantum to classical environment. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 6748-6753.	7.1	22
13	Optimized effective potential using the Hylleraas variational method. Physical Review B, 2012, 85, .	3.2	19
14	Progress at the interface of wave-function and density-functional theories. Physical Review A, 2011, 83, .	2.5	17
15	Density-inversion method for the Kohnâ€“Sham potential: Role of the screening density. Journal of Chemical Physics, 2020, 152, 164114.	3.0	17
16	Density functional theory for excited states. International Journal of Quantum Chemistry, 1995, 56, 333-336.	2.0	16
17	Quasi-particle energy spectra in local reduced density matrix functional theory. Journal of Chemical Physics, 2014, 141, 164120.	3.0	15
18	Constrained optimized potential method and secondâ€order correlation energy for excited states. International Journal of Quantum Chemistry, 2007, 107, 2604-2615.	2.0	13

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19	Distinct Magnetic Phase Transition at the Surface of an Antiferromagnet. Physical Review Letters, 2014, 112, 167201.	7.8	10
20	Orbitals from local RDMFT: Are they Kohn-Sham or natural orbitals?. Journal of Chemical Physics, 2015, 143, 054106.	3.0	10
21	The Statistical Distribution Function For An Anyon Liquid. Physics and Chemistry of Liquids, 1993, 26, 135-141.	1.2	9
22	Reply to â€œComment on â€˜Nonanalyticity of the optimized effective potential with finite basis setsâ€™â€‰â€. Physical Review A, 2013, 88, .	2.5	8
23	Performance of the constrained minimization of the total energy in density functional approximations: the electron repulsion density and potential. European Physical Journal B, 2018, 91, 1.	1.5	8
24	Effect of quantization of vibrations on the structural properties of crystals. Physical Review B, 2008, 78, .	3.2	7
25	General local and rectilinear vibrational coordinates consistent with Eckartâ€™s conditions. Physical Review A, 2009, 79, .	2.5	7
26	Alternative Technique for the Constrained Variational Problem Based on an Asymptotic Projection Method: I. Basics. Progress in Theoretical Chemistry and Physics, 2008, , 429-450.	0.2	7
27	A correction for the Hartree-Fock density of states for jellium without screening. Journal of Chemical Physics, 2015, 142, 084116.	3.0	6
28	Excitation Energies of Molecules from Ensemble Density Functional Theory. Advances in Quantum Chemistry, 2016, , 199-229.	0.8	6
29	Alternative Technique for the Constrained Variational Problem Based on an Asymptotic Projection Method: II. Applications to Open-Shell Self-Consistent Field Theory. Progress in Theoretical Chemistry and Physics, 2008, , 451-489.	0.2	6
30	Self-consistent geometry in the computation of the vibrational spectra of molecules. Physical Review A, 2009, 80, .	2.5	5
31	Comment on â€œHigh-energy neutron scattering from hydrogen using a direct geometry spectrometerâ€. Physical Review B, 2011, 84, .	3.2	5
32	Dynamics of Open Quantum Systems Using Parametric Representation with Coherent States. Open Systems and Information Dynamics, 2013, 20, 1340002.	1.2	5
33	Constrained Local Potentials for Self-Interaction Correction. Advances in Atomic, Molecular and Optical Physics, 2015, 64, 129-142.	2.3	5
34	Optimal power series expansions of the Kohnâ€“Sham potential. European Physical Journal B, 2018, 91, 1.	1.5	5
35	Improving the exchange and correlation potential in density-functional approximations through constraints. Faraday Discussions, 2020, 224, 126-144.	3.2	5
36	Exactly Solvable Model Mimicking the H2 Molecule in the Limit of Large Nuclear Masses. Journal of Mathematical Chemistry, 2007, 42, 603-615.	1.5	4

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37	Hohenberg-Kohn Theorem and Constrained Search Formulation for Diagonal Spin Density Functional Theory. Progress in Theoretical Chemistry and Physics, 2003, , 195-205.	0.2	3
38	Generalised Kohn-Sham equations with accurate total energy and single-particle eigenvalue spectrum. Journal of Chemical Physics, 2021, 155, 224105.	3.0	3
39	Density functionals with spin-density accuracy for open shells. Journal of Chemical Physics, 2022, 156, 111101.	3.0	3
40	On the treatment of singularities of the Watson Hamiltonian for nonlinear molecules. International Journal of Quantum Chemistry, 2011, 111, 307-317.	2.0	2
41	Open Quantum Systems and the Parametric Representation: From Entanglement to Berryâ€™s Phase. International Journal of Theoretical Physics, 2014, 53, 3434-3446.	1.2	2
42	Challenges for large scale simulation: general discussion. Faraday Discussions, 2020, 224, 309-332.	3.2	2
43	Strong correlation in density functional theory: general discussion. Faraday Discussions, 2020, 224, 373-381.	3.2	2
44	New approaches to study excited states in density functional theory: general discussion. Faraday Discussions, 2020, 224, 483-508.	3.2	2
45	Second virial coefficient of the interacting anyon gas. Physical Review B, 1994, 49, 6808-6814.	3.2	1
46	Low excitations of the anyon gas. Journal of Physics Condensed Matter, 1995, 7, L239-L244.	1.8	1
47	New density-functional approximations and beyond: general discussion. Faraday Discussions, 2020, 224, 166-200.	3.2	1
48	Enhanced electronâ€“phonon coupling near an electronic quantum phase transition. Journal of Physics Condensed Matter, 2022, 34, 14LT01.	1.8	1
49	Nuclear Quantum Effects on the Structural Properties of Solids. AIP Conference Proceedings, 2007, , .	0.4	0
50	Unconstrained Variational Determination of the Kohn-Sham Potential. , 2006, , 1469-1472.		0