Anouar Benali

List of Publications by Year
in descending order

35 papers	956 citations	516710 16 h-index	434195 31 g-index
35 all docs	35 docs citations	35 times ranked	1063 citing authors

#	Article	IF	Citations
1	<tt>QMCPACK</tt>: an open sourceab initioquantum Monte Carlo package for the electronic structure of atoms, molecules and solids. Journal of Physics Condensed Matter, 2018, 30, 195901.	1.8	187
2	Quantum Package 2.0: An Open-Source Determinant-Driven Suite of Programs. Journal of Chemical Theory and Computation, 2019, 15, 3591-3609.	5.3	108
3	QMCPACK: Advances in the development, efficiency, and application of auxiliary field and real-space variational and diffusion quantum Monte Carlo. Journal of Chemical Physics, 2020, 152, 174105.	3.0	80
4	Benchmarks and Reliable DFT Results for Spin Gaps of Small Ligand Fe(II) Complexes. Journal of Chemical Theory and Computation, 2018, 14, 2304-2311.	5.3	71
5	Application of Diffusion Monte Carlo to Materials Dominated by van der Waals Interactions. Journal of Chemical Theory and Computation, 2014, 10, 3417-3422.	5.3	67
6	Phase stability of TiO₂polymorphs from diffusion Quantum Monte Carlo. New Journal of Physics, 2016, 18, 113049.	2.9	59
7	Excitation energies from diffusion Monte Carlo using selected configuration interaction nodes. Journal of Chemical Physics, 2018, 149, 034108.	3.0	50
8	Electronic properties of doped and defective NiO: A quantum Monte Carlo study. Physical Review Materials, 2017, 1, .	2.4	36
9	Quantum Monte Carlo analysis of a charge ordered insulating antiferromagnet: the Ti₄O₇ MagnÃ©li phase. Physical Chemistry Chemical Physics, 2016, 18, 18323-18335.	2.8	27
10	Nature of Interlayer Binding and Stacking of spâ€“sp² Hybridized Carbon Layers: A Quantum Monte Carlo Study. Journal of Chemical Theory and Computation, 2017, 13, 5639-5646.	5.3	27
11	Density functional study of copper segregation in aluminum. Surface Science, 2011, 605, 341-350.	1.9	24
12	Phase stability and interlayer interaction of blue phosphorene. Physical Review B, 2018, 98, .	3.2	19
13	Influence of pseudopotentials on excitation energies from selected configuration interaction and diffusion Monte Carlo. Results in Chemistry, 2019, 1, 100002.	2.0	18
14	Doped NiO: The mottness of a charge transfer insulator. Physical Review B, 2020, 101, .	3.2	16
15	Optimized structure and electronic band gap of monolayer GeSe from quantum Monte Carlo methods. Physical Review Materials, 2021, 5, .	2.4	16
16	Toward a systematic improvement of the fixed-node approximation in diffusion Monte Carlo for solidsâ€”A case study in diamond. Journal of Chemical Physics, 2020, 153, 184111.	3.0	16
17	Zirconia and hafnia polymorphs: Ground-state structural properties from diffusion Monte Carlo. Physical Review Materials, 2018, 2, .	2.4	16
18	Quantum Monte Carlo benchmarking of large noncovalent complexes in the L7 benchmark set. Journal of Chemical Physics, 2020, 153, 194113.	3.0	14

#	Article	IF	Citations
19	Systematic comparison and cross-validation of fixed-node diffusion Monte Carlo and phaseless auxiliary-field quantum Monte Carlo in solids. Physical Review B, 2020, 102, .	3.2	13
20	Competition between HÃ¼ckelâ€™s Rule and Jahnâ€“Teller Distortion in Small Carbon Rings: A Quantum Monte Carlo Study. Journal of Physical Chemistry A, 2020, 124, 3636-3640.	2.5	13
21	Importance of Van der Waals Interactions in Hydrogen Adsorption on a Silicon-carbide Nanotube Revisited with vdW-DFT and Quantum Monte Carlo. ACS Omega, 2021, 6, 24630-24636.	3.5	12
22	Taming the fixed-node error in diffusion Monte Carlo via range separation. Journal of Chemical Physics, 2020, 153, 174107.	3.0	11
23	Ti interstitial flows giving rutile TiO2 reoxidation process enhancement in (001) surface. Physical Review Materials, 2019, 3, .	2.4	7
24	Quantum Monte Carlo Calculations of Catalytic Energy Barriers in a Metallorganic Framework with Transition-Metal-Functionalized Nodes. Journal of Physical Chemistry C, 2018, 122, 16683-16691.	3.1	6
25	Diffusion Monte Carlo study of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> adsorption on single layer graphene. Physical Review B, 2019, 100, .	3.2	6
26	Local structure of potassium doped nickel oxide: A combined experimental-theoretical study. Physical Review Materials, 2019, 3, .	2.4	6
27	Energetic Stability of Free-standing and Metal-Supported Borophenes: Quantum Monte Carlo and Density Functional Theory Calculations. Journal of Physical Chemistry C, 2020, 124, 24420-24428.	3.1	5
28	Defect energetics of cubic hafnia from quantum Monte Carlo simulations. Physical Review Materials, 2019, 3, .	2.4	5
29	Embracing a new era of highly efficient and productive quantum Monte Carlo simulations. , 2017, , .		4
30	Metastable Metallic Phase of a Bilayer Blue Phosphorene Induced by Interlayer Bonding and Intralayer Charge Redistributions. Journal of Physical Chemistry Letters, 2021, 12, 10981-10986.	4.6	4
31	Globalâ€view coefficients: a data management solution for parallel quantum Monte Carlo applications. Concurrency Computation Practice and Experience, 2016, 28, 3655-3671.	2.2	3
32	Adsorption of a single Pt atom on graphene: spin crossing between physisorbed triplet and chemisorbed singlet states. Physical Chemistry Chemical Physics, 2021, 23, 22147-22154.	2.8	3
33	The binding of atomic hydrogen on graphene from density functional theory and diffusion Monte Carlo calculations. Journal of Chemical Physics, 2022, 156, 144702.	3.0	3
34	Optimization and Parallelization of B-Spline Based Orbital Evaluations in QMC on Multi/Many-Core Shared Memory Processors. , 2017, , .		2
35	Assessing the accuracy of compound formation energies with quantum Monte Carlo. Physical Review B, 2022, 105, .	3.2	2