

Anouar Benali

List of Publications by Year in descending order

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35
papers

956
citations

516710

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434195

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docs citations

35
times ranked

1063
citing authors

#	ARTICLE	IF	CITATIONS
1	The binding of atomic hydrogen on graphene from density functional theory and diffusion Monte Carlo calculations. <i>Journal of Chemical Physics</i> , 2022, 156, 144702.	3.0	3
2	Assessing the accuracy of compound formation energies with quantum Monte Carlo. <i>Physical Review B</i> , 2022, 105, .	3.2	2
3	Adsorption of a single Pt atom on graphene: spin crossing between physisorbed triplet and chemisorbed singlet states. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 22147-22154.	2.8	3
4	Optimized structure and electronic band gap of monolayer GeSe from quantum Monte Carlo methods. <i>Physical Review Materials</i> , 2021, 5, .	2.4	16
5	Importance of Van der Waals Interactions in Hydrogen Adsorption on a Silicon-carbide Nanotube Revisited with vdW-DFT and Quantum Monte Carlo. <i>ACS Omega</i> , 2021, 6, 24630-24636.	3.5	12
6	Metastable Metallic Phase of a Bilayer Blue Phosphorene Induced by Interlayer Bonding and Intralayer Charge Redistributions. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 10981-10986.	4.6	4
7	Systematic comparison and cross-validation of fixed-node diffusion Monte Carlo and phaseless auxiliary-field quantum Monte Carlo in solids. <i>Physical Review B</i> , 2020, 102, .	3.2	13
8	Quantum Monte Carlo benchmarking of large noncovalent complexes in the L7 benchmark set. <i>Journal of Chemical Physics</i> , 2020, 153, 194113.	3.0	14
9	Energetic Stability of Free-standing and Metal-Supported Borophenes: Quantum Monte Carlo and Density Functional Theory Calculations. <i>Journal of Physical Chemistry C</i> , 2020, 124, 24420-24428.	3.1	5
10	Doped NiO: The mottness of a charge transfer insulator. <i>Physical Review B</i> , 2020, 101, .	3.2	16
11	QMCPACK: Advances in the development, efficiency, and application of auxiliary field and real-space variational and diffusion quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2020, 152, 174105.	3.0	80
12	Competition between Hückel's Rule and Jahn-Teller Distortion in Small Carbon Rings: A Quantum Monte Carlo Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3636-3640.	2.5	13
13	Toward a systematic improvement of the fixed-node approximation in diffusion Monte Carlo for solids: A case study in diamond. <i>Journal of Chemical Physics</i> , 2020, 153, 184111.	3.0	16
14	Taming the fixed-node error in diffusion Monte Carlo via range separation. <i>Journal of Chemical Physics</i> , 2020, 153, 174107.	3.0	11
15	Influence of pseudopotentials on excitation energies from selected configuration interaction and diffusion Monte Carlo. <i>Results in Chemistry</i> , 2019, 1, 100002.	2.0	18
16	Diffusion Monte Carlo study of O_2 adsorption on single layer graphene. <i>Physical Review B</i> , 2019, 100, .	3.2	6
17	Quantum Package 2.0: An Open-Source Determinant-Driven Suite of Programs. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3591-3609.	5.3	108
18	Defect energetics of cubic hafnia from quantum Monte Carlo simulations. <i>Physical Review Materials</i> , 2019, 3, .	2.4	5

#	ARTICLE	IF	CITATIONS
19	Local structure of potassium doped nickel oxide: A combined experimental-theoretical study. Physical Review Materials, 2019, 3, .	2.4	6
20	Ti interstitial flows giving rutile TiO ₂ reoxidation process enhancement in (001) surface. Physical Review Materials, 2019, 3, .	2.4	7
21	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
22	QMCPACK: an open source ab initio quantum Monte Carlo package for the electronic structure of atoms, molecules and solids. Journal of Physics Condensed Matter, 2018, 30, 195901.	1.8	187
23	Excitation energies from diffusion Monte Carlo using selected configuration interaction nodes. Journal of Chemical Physics, 2018, 149, 034108.	3.0	50
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	Phase stability and interlayer interaction of blue phosphorene. Physical Review B, 2018, 98, .	3.2	19
26	Zirconia and hafnia polymorphs: Ground-state structural properties from diffusion Monte Carlo. Physical Review Materials, 2018, 2, .	2.4	16
27	Nature of Interlayer Binding and Stacking of sp ² Hybridized Carbon Layers: A Quantum Monte Carlo Study. Journal of Chemical Theory and Computation, 2017, 13, 5639-5646.	5.3	27
28	Embracing a new era of highly efficient and productive quantum Monte Carlo simulations. , 2017, , .		4
29	Optimization and Parallelization of B-Spline Based Orbital Evaluations in QMC on Multi/Many-Core Shared Memory Processors. , 2017, , .		2
30	Electronic properties of doped and defective NiO: A quantum Monte Carlo study. Physical Review Materials, 2017, 1, .	2.4	36
31	Global 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	Phase stability of TiO ₂ polymorphs from diffusion Quantum Monte Carlo. New Journal of Physics, 2016, 18, 113049.	2.9	59
33	Quantum Monte Carlo analysis of a charge ordered insulating antiferromagnet: the Ti ₄ O ₇ Magnéli phase. Physical Chemistry Chemical Physics, 2016, 18, 18323-18335.	2.8	27
34	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
35	Density functional study of copper segregation in aluminum. Surface Science, 2011, 605, 341-350.	1.9	24