Nikolay A Bogdanov

List of Publications by Year
in descending order

24 papers	1,813 citations	516710 16 h-index	642732 23 g-index
29 all docs	29 docs citations	29 times ranked	2235 citing authors

#	Article	IF	Citations
1	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
2	Recent developments in the P<scp>y</scp>SCF program package. Journal of Chemical Physics, 2020, 153, 024109.	3.0	388
3	Kitaev exchange and field-induced quantum spin-liquid states in honeycomb Î±-RuCl3. Scientific Reports, 2016, 6, 37925.	3.3	215
4	Orbital reconstruction in nonpolar tetravalent transition-metal oxide layers. Nature Communications, 2015, 6, 7306.	12.8	60
5	Magnetic State of PyrochloreCd2Os2O7Emerging from Strong Competition of Ligand Distortions and Longer-Range Crystalline Anisotropy. Physical Review Letters, 2013, 110, 127206.	7.8	59
6	Spin-orbit-driven magnetic structure and excitation in the 5d pyrochlore Cd2Os2O7. Nature Communications, 2016, 7, 11651.	12.8	56
7	NECI: N-Electron Configuration Interaction with an emphasis on state-of-the-art stochastic methods. Journal of Chemical Physics, 2020, 153, 034107.	3.0	55
8	Post-perovskite CaIrO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>: A<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="bold-italic">j</mml:mi><mml:mo>=</mml:mo><mml:mn mathvariant="bold">1</mml:mn><mml:mo>/</mml:mo><mml:mn mathvariant="bold">2</mml:mn></mml:mrow></mml:math> Mott insulator. Physical Review B, 2014, 89, .	3.2	45
9	Electronic correlations and magnetic interactions in infinite-layer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>NdNiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2020, 102, .	3.2	38
10	Ab initiocalculation ofd-dexcitations in quasi-one-dimensional Cud9correlated materials. Physical Review B, 2011, 84, .	3.2	29
11	Observation of heavy spin-orbit excitons propagating in a nonmagnetic background: The case of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow><mml:mo>(</mml:mo><mml:mi>Ba</mml:mi> Physical Review B, 2018, 97, .	3.2	29
12	Spin-Pure Stochastic-CASSCF via GUGA-FCIQMC Applied to Ironâ€“Sulfur Clusters. Journal of Chemical Theory and Computation, 2021, 17, 5684-5703.	5.3	25
13	Strongly gapped spin-wave excitation in the insulating phase of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="bold">NaOsO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2017, 95, .	3.2	24
14	Resolution of Low-Energy States in Spin-Exchange Transition-Metal Clusters: Case Study of Singlet States in [Fe(III)₄S₄] Cubanes. Journal of Physical Chemistry A, 2021, 125, 4727-4740.	2.5	22
15	Heavy-mass magnetic modes in pyrochlore iridates due to dominant Dzyaloshinskii-Moriya interaction. Physical Review Materials, 2018, 2, .	2.4	20
16	Covalency and vibronic couplings make a nonmagnetic j=3/2 ion magnetic. Npj Quantum Materials, 2016, 1, .	5.2	19
17	The color center singlet state of oxygen vacancies in TiO2. Journal of Chemical Physics, 2020, 153, 204704.	3.0	13
18	Ab initiocomputation of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>d</mml:mi></mml:math>-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>d</mml:mi></mml:math>excitation energies in low-dimensional Ti and V oxychlorides. Physical Review B, 2011, 84, .	3.2	11

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19	A full configuration interaction quantum Monte Carlo study of ScO, TiO, and VO molecules. Journal of Chemical Physics, 2021, 154, 164302.	3.0	11
20	Enhancement of superexchange due to synergetic breathing and hopping in corner-sharing cuprates. Nature Physics, 2022, 18, 190-195.	16.7	10
21	Combined unitary and symmetric group approach applied to low-dimensional Heisenberg spin systems. Physical Review B, 2022, 105, .	3.2	9
22	Orbital breathing effects in the computation of x-rayd-ion spectra in solids byab initiowave-function-based methods. Journal of Physics Condensed Matter, 2017, 29, 035502.	1.8	5
23	Spin and orbital excitations through the metal-to-insulator transition in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Cd</mml:mi><mml:mn>2</mml:mn></mml: mathvariant="normal">O</mml:mi><mml:mn>7</mml:mn></mml:msub></mml:mrow></mml:math> probed with high-resolution resonant inelastic x-ray scattering. Physical Review B, 2020, 101, .	3.2	5
24	Ab Initio Wavefunction Analysis of Electron Removal Quasi-Particle State of NdNiO2 With Fully Correlated Quantum Chemical Methods. Frontiers in Physics, 2022, 10, .	2.1	0