Carlos A JimÃ©nez-Hoyos

List of Publications by Year
in descending order

36 papers	1,244 citations	361413 20 h-index	361022 35 g-index
36 all docs	36 docs citations	36 times ranked	1066 citing authors

#	Article	IF	Citations
1	Ground states of Heisenberg spin clusters from projected Hartree-Fock theory. Physical Review B, 2022, 105, .	3.2	3
2	Prediction of Fluorophore Brightness in Designed Mini Fluorescence Activating Proteins. Journal of Chemical Theory and Computation, 2022, 18, 3190-3203.	5.3	0
3	Coupled Cluster and Perturbation Theories Based on a Cluster Mean-Field Reference Applied to Strongly Correlated Spin Systems. Journal of Chemical Theory and Computation, 2022, 18, 4293-4303.	5.3	8
4	Electronic Spectroscopy of 2-Phenyl-1,3,2-benzodioxaborole and Its Derivatives: Important Building Blocks of Covalent Organic Frameworks. Journal of Physical Chemistry A, 2020, 124, 529-537.	2.5	1
5	Hyperfine-Coupling Tensors from Projected Hartreeâ€“Fock Theory. Journal of Chemical Theory and Computation, 2020, 16, 6222-6235.	5.3	3
6	Ground-State Properties of the Hydrogen Chain: Dimerization, Insulator-to-Metal Transition, and Magnetic Phases. Physical Review X, 2020, 10, .	8.9	42
7	Minimal Matrix Product States and Generalizations of Mean-Field and Geminal Wave Functions. Journal of Chemical Theory and Computation, 2020, 16, 5057-5066.	5.3	7
8	Approaching the full configuration interaction ground state from an arbitrary wavefunction with gradient descent and quasi-Newton algorithms. Journal of Chemical Physics, 2020, 153, 234113.	3.0	1
9	Low-Cost Molecular Excited States from a State-Averaged Resonating Hartreeâ€“Fock Approach. Journal of Chemical Theory and Computation, 2019, 15, 5343-5351.	5.3	11
10	Coupled-cluster impurity solvers for dynamical mean-field theory. Physical Review B, 2019, 100, .	3.2	37
11	Efficient Implementation of Variation after Projection Generalized Hartreeâ€“Fock. Journal of Chemical Theory and Computation, 2018, 14, 588-596.	5.3	14
12	Magnetic Structure of Density Matrices. Journal of Chemical Theory and Computation, 2018, 14, 649-659.	5.3	12
13	Lie algebraic similarity transformed Hamiltonians for lattice model systems. Physical Review B, 2015, 91, .	3.2	23
14	Cluster-based mean-field and perturbative description of strongly correlated fermion systems: Application to the one- and two-dimensional Hubbard model. Physical Review B, 2015, 92, .	3.2	20
15	Analytic energy gradient for the projected Hartreeâ€“Fock method. Journal of Chemical Physics, 2014, 140, 204101.	3.0	15
16	Symmetry-projected wave functions in quantum Monte Carlo calculations. Physical Review B, 2014, 89, .	3.2	43
17	Variational description of the ground state of the repulsive two-dimensional Hubbard model in terms of nonorthogonal symmetry-projected Slater determinants. Physical Review B, 2014, 90, .	3.2	11
18	Multireference symmetry-projected variational approximation for the ground state of the doped one-dimensional Hubbard model. Physical Review B, 2014, 89, .	3.2	7

#	Article	IF	Citations
19	Potential energy curves for Mo₂: multi-component symmetry-projected Hartreeâ€“Fock and beyond. Molecular Physics, 2014, 112, 1938-1946.	1.7	9
20	Electronic correlation without double counting via a combination of spin projected Hartree-Fock and density functional theories. Journal of Chemical Physics, 2014, 140, 244102.	3.0	26
21	Polyradical Character and Spin Frustration in Fullerene Molecules: An Ab Initio Non-Collinear Hartreeâ€“Fock Study. Journal of Physical Chemistry A, 2014, 118, 9925-9940.	2.5	43
22	Stability of Hemi-Bonded vs Proton-Transferred Structures of (H₂O)₂⁺, (H₂S)₂⁺, and (H₂Se)₂⁺ Studied with Projected Hartreeâ€“Fock Methods. Journal of Physical Chemistry A, 2014, 118, 7261-7266.	2.5	26
23	Entanglement and Polyradical Character of Polycyclic Aromatic Hydrocarbons Predicted by Projected Hartreeâ€“Fock Theory. Journal of Physical Chemistry B, 2013, 117, 12750-12758.	2.6	82
24	Excited electronic states from a variational approach based on symmetry-projected Hartreeâ€“Fock configurations. Journal of Chemical Physics, 2013, 139, 224110.	3.0	28
25	Predicting Singletâ€“Triplet Energy Splittings with Projected Hartreeâ€“Fock Methods. Journal of Physical Chemistry A, 2013, 117, 8073-8080.	2.5	29
26	Multi-component symmetry-projected approach for molecular ground state correlations. Journal of Chemical Physics, 2013, 139, 204102.	3.0	51
27	Multireference symmetry-projected variational approaches for ground and excited states of the one-dimensional Hubbard model. Physical Review B, 2013, 87, .	3.2	44
28	Symmetry-projected variational approach for ground and excited states of the two-dimensional Hubbard model. Physical Review B, 2012, 85, .	3.2	42
29	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>N</mml:mi></mml:math>-electron Slater determinants from nonunitary canonical transformations of fermion operators. Physical Review A, 2012, 86, .	2.5	14
30	Exploring Copper Oxide Cores Using the Projected Hartreeâ€“Fock Method. Journal of Chemical Theory and Computation, 2012, 8, 4944-4949.	5.3	33
31	Projected Hartreeâ€“Fock theory. Journal of Chemical Physics, 2012, 136, 164109.	3.0	191
32	Generalized Hartreeâ€“Fock Description of Molecular Dissociation. Journal of Chemical Theory and Computation, 2011, 7, 2667-2674.	5.3	64
33	Projected quasiparticle theory for molecular electronic structure. Journal of Chemical Physics, 2011, 135, 124108.	3.0	148
34	Evaluation of Range-Separated Hybrid and Other Density Functional Approaches on Test Sets Relevant for Transition Metal-Based Homogeneous Catalysts. Journal of Physical Chemistry A, 2009, 113, 11742-11749.	2.5	50
35	Assessment of a density functional with full exact exchange and balanced non-locality of correlation. Molecular Physics, 2009, 107, 1077-1088.	1.7	17
36	Evaluation of range-separated hybrid density functionals for the prediction of vibrational frequencies, infrared intensities, and Raman activities. Physical Chemistry Chemical Physics, 2008, 10, 6621.	2.8	89