Zhenhua Chen

List of Publications by Year
in descending order

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		759233	713466
25	431	12	21
papers	citations	h-index	g-index

25	25	25	245
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Compact and accurate ab initio valence bond wave functions for electron transfer: The classic but challenging covalent-ionic interaction in LiF. Journal of Chemical Physics, 2022, 157, .	3.0	3
2	Valence Bond Alternative Yielding Compact and Accurate Wave Functions for Challenging Excited States. Application to Ozone and Sulfur Dioxide. Journal of Chemical Theory and Computation, 2021, 17, 330-343.	5.3	10
3	N-Body Reduced Density Matrix-Based Valence Bond Theory and Its Applications in Diabatic Electronic-Structure Computations. Accounts of Chemical Research, 2021, 54, 3895-3905.	15.6	3
4	Extended Mullikenâ€“Hush Method with Applications to the Theoretical Study of Electron Transfer. Journal of Chemical Theory and Computation, 2021, 17, 6861-6875.	5.3	3
5	Ab initio valence bond theory: A brief history, recent developments, and near future. Journal of Chemical Physics, 2020, 153, 090902.	3.0	26
6	Graphical Representation of HÃ¼ckel Molecular Orbitals. Journal of Chemical Education, 2020, 97, 448-456.	2.3	3
7	Two-Dimensional Analysis of the Diabatic Transition of a General Vectorial Physical Observable Based on Adiabatic-to-Diabatic Transformation. Journal of Physical Chemistry Letters, 2019, 10, 5868-5872.	4.6	6
8	Novel implementation of seniority number truncated valence bond methods with applications to H22 chain. Journal of Chemical Physics, 2019, 151, 194107.	3.0	5
9	Reciprocal transformation of seniority number restricted wave function. Journal of Chemical Physics, 2018, 149, 044111.	3.0	4
10	Explicit construction of diabatic state and its application to the direct evaluation of electronic coupling. Journal of Chemical Physics, 2018, 149, 044112.	3.0	13
11	The driving force for Î-bond localization and bond alternation in trisannelated benzenes. Physical Chemistry Chemical Physics, 2017, 19, 3019-3027.	2.8	1
12	A comparative study on seniority-based MO and VB calculations of the singlet and triplet energy gaps of open-shell molecules. Computational and Theoretical Chemistry, 2017, 1116, 86-91.	2.5	5
13	The application of cholesky decomposition in valence bond calculation. Journal of Computational Chemistry, 2016, 37, 2157-2162.	3.3	5
14	Seniority Number in Valence Bond Theory. Journal of Chemical Theory and Computation, 2015, 11, 4102-4108.	5.3	17
15	XMVB 2.0: A new version of Xiamen valence bond program. International Journal of Quantum Chemistry, 2015, 115, 731-737.	2.0	65
16	Nonorthogonal orbital based n-body reduced density matrices and their applications to valence bond theory. III. Second-order perturbation theory using valence bond self-consistent field function as reference. Journal of Chemical Physics, 2014, 141, 134118.	3.0	32
17	Nonorthogonal orbital based N-body reduced density matrices and their applications to valence bond theory. IV. The automatic implementation of the Hessian based VBSCF method. Journal of Chemical Physics, 2014, 141, 194113.	3.0	17
18	GVVPT2 multireference perturbation theory study of selenium oxides. Molecular Physics, 2013, 111, 1078-1091.	1.7	4

#	Article	IF	Citations
19	Nonorthogonal orbital basedN-body reduced density matrices and their applications to valence bond theory. I. Hamiltonian matrix elements between internally contracted excited valence bond wave functions. Journal of Chemical Physics, 2013, 138, 164119.	3.0	31
20	An efficient algorithm for complete active space valence bond selfâ€consistent field calculation. Journal of Computational Chemistry, 2013, 34, 38-48.	3.3	12
21	Nonorthogonal orbital based N-body reduced density matrices and their applications to valence bond theory. II. An efficient algorithm for matrix elements and analytical energy gradients in VBSCF method. Journal of Chemical Physics, 2013, 138, 164120.	3.0	42
22	DFVB: A Density-Functional-Based Valence Bond Method. Journal of Chemical Theory and Computation, 2012, 8, 1608-1615.	5.3	38
23	Orbitally invariant internally contracted multireference unitary coupled cluster theory and its perturbative approximation: Theory and test calculations of second order approximation. Journal of Chemical Physics, 2012, 137, 014108.	3.0	39
24	A new algorithm for inactive orbital optimization in valence bond theory. Science in China Series B: Chemistry, 2009, 52, 1879-1884.	0.8	4
25	Valence Bond Perturbation Theory. A Valence Bond Method That Incorporates Perturbation Theory. Journal of Physical Chemistry A, 2009, 113, 11560-11569.	2.5	43