

Ida-Marie HÃyvik

List of Publications by Year in descending order

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Version: 2024-02-01

24
papers

1,821
citations

687363

13
h-index

642732

23
g-index

24
all docs

24
docs citations

24
times ranked

1991
citing authors

#	ARTICLE	IF	CITATIONS
1	The Dalton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	14.6	1,166
2	The divide-expand-consolidate family of coupled cluster methods: Numerical illustrations using second order Møller-Plesset perturbation theory. Journal of Chemical Physics, 2012, 136, 014105.	3.0	80
3	Orbital localization using fourth central moment minimization. Journal of Chemical Physics, 2012, 137, 224114.	3.0	71
4	CT1.0: An open source electronic structure program with emphasis on coupled cluster and multilevel methods. Journal of Chemical Physics, 2020, 152, 184103.	3.0	68
5	Trust Region Minimization of Orbital Localization Functions. Journal of Chemical Theory and Computation, 2012, 8, 3137-3146.	5.3	64
6	MP2 energy and density for large molecular systems with internal error control using the Divide-Expand-Consolidate scheme. Physical Chemistry Chemical Physics, 2012, 14, 15706.	2.8	57
7	Characterization and Generation of Local Occupied and Virtual Hartree-Fock Orbitals. Chemical Reviews, 2016, 116, 3306-3327.	47.7	48
8	Pipek-Mezey localization of occupied and virtual orbitals. Journal of Computational Chemistry, 2013, 34, 1456-1462.	3.3	43
9	The divide-expand-consolidate MP2 scheme goes massively parallel. Molecular Physics, 2013, 111, 1196-1210.	1.7	38
10	Potential Energy Surfaces for Vibrational Structure Calculations from a Multiresolution Adaptive Density-Guided Approach: Implementation and Test Calculations. Journal of Physical Chemistry A, 2009, 113, 8712-8723.	2.5	34
11	Correlated natural transition orbitals for core excitation energies in multilevel coupled cluster models. Journal of Chemical Physics, 2017, 146, 144109.	3.0	31
12	Density-Based Multilevel Hartree-Fock Model. Journal of Chemical Theory and Computation, 2017, 13, 5282-5290.	5.3	30
13	A perspective on the localizability of Hartree-Fock orbitals. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	25
14	Convergence acceleration for the multilevel Hartree-Fock model. Molecular Physics, 2020, 118, 1626929.	1.7	11
15	Local Hartree-Fock orbitals using a three-level optimization strategy for the energy. Journal of Computational Chemistry, 2013, 34, 1311-1320.	3.3	10
16	Localized orbitals from basis sets augmented with diffuse functions. Journal of Chemical Physics, 2013, 138, 204104.	3.0	9
17	Generalising localisation schemes of orthogonal orbitals to the localisation of non-orthogonal orbitals. Molecular Physics, 2017, 115, 16-25.	1.7	8
18	The spectrum of the atomic orbital overlap matrix and the locality of the virtual electronic density matrix. Molecular Physics, 2020, 118, e1765034.	1.7	7

#	ARTICLE	IF	CITATIONS
19	Unimolecular Decomposition Reactions of Picric Acid and Its Methylated Derivativesâ”€A DFT Study. Journal of Physical Chemistry A, 2022, 126, 2645-2657.	2.5	5
20	Tautomerization of Thymine Using Ultraviolet Light. Langmuir, 2017, 33, 9666-9672.	3.5	4
21	Describing ground and excited state potential energy surfaces for molecular photoswitches using coupled cluster models. Journal of Computational Chemistry, 2021, 42, 1419-1429.	3.3	4
22	Linear-Scaling Implementation of Multilevel Hartreeâ”€Fock Theory. Journal of Chemical Theory and Computation, 2021, 17, 7416-7427.	5.3	4
23	The effect of midbond functions on interaction energies computed using <sc>MP2</sc> and <sc>CCSD</sc>(T). Journal of Computational Chemistry, 2022, 43, 121-131.	3.3	4
24	Convergence of the electronic density for a target region in cluster models of a NH ₃ molecular crystal. Journal of Mathematical Chemistry, 0, , .	1.5	0