Andreas HeÃelmann

List of Publications by Year
in descending order

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50	3,787	186265 28	189892 50
papers	citations	h-index	g-index

52	52	52	2165
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The Molpro quantum chemistry package. Journal of Chemical Physics, 2020, 152, 144107.	3.0	603
2	Intermolecular dispersion energies from time-dependent density functional theory. Chemical Physics Letters, 2003, 367, 778-784.	2.6	358
3	First-order intermolecular interaction energies from Kohnâ€“Sham orbitals. Chemical Physics Letters, 2002, 357, 464-470.	2.6	323
4	Intermolecular induction and exchange-induction energies from coupled-perturbed Kohnâ€“Sham density functional theory. Chemical Physics Letters, 2002, 362, 319-325.	2.6	240
5	The helium dimer potential from a combined density functional theory and symmetry-adapted perturbation theory approach using an exact exchangeâ€“correlation potential. Physical Chemistry Chemical Physics, 2003, 5, 5010-5014.	2.8	198
6	Interaction Energy Contributions of H-Bonded and Stacked Structures of the AT and GC DNA Base Pairs from the Combined Density Functional Theory and Intermolecular Perturbation Theory Approach. Journal of the American Chemical Society, 2006, 128, 11730-11731.	13.7	181
7	Comment on â€œUsing Kohnâ^'Sham Orbitals in Symmetry-Adapted Perturbation Theory To Investigate Intermolecular Interactionsâ€• Journal of Physical Chemistry A, 2001, 105, 11156-11157.	2.5	165
8	Accurate Intermolecular Interaction Energies from a Combination of MP2 and TDDFT Response Theory. Journal of Chemical Theory and Computation, 2010, 6, 168-178.	5.3	154
9	Numerically stable optimized effective potential method with balanced Gaussian basis sets. Journal of Chemical Physics, 2007, 127, 054102.	3.0	130
10	Improved supermolecular second order MÃ¸llerâ€“Plesset intermolecular interaction energies using time-dependent density functional response theory. Journal of Chemical Physics, 2008, 128, 144112.	3.0	123
11	Random phase approximation correlation energies with exact Kohnâ€“Sham exchange. Molecular Physics, 2010, 108, 359-372.	1.7	121
12	Symmetry-Adapted Perturbation Theory Applied to Endohedral Fullerene Complexes: A Stability Study of H₂@C₆₀ and 2H₂@C₆₀. Journal of Chemical Theory and Computation, 2009, 5, 1585-1596.	5.3	83
13	On the accuracy of DFT-SAPT, MP2, SCS-MP2, MP2C, and DFT+Disp methods for the interaction energies of endohedral complexes of the C₆₀fullerene with a rare gas atom. Physical Chemistry Chemical Physics, 2011, 13, 732-743.	2.8	82
14	Efficient self-consistent treatment of electron correlation within the random phase approximation. Journal of Chemical Physics, 2013, 139, 084113.	3.0	81
15	Intermolecular symmetry-adapted perturbation theory study of large organic complexes. Journal of Chemical Physics, 2014, 141, 094107.	3.0	77
16	Directional Noncovalent Interactions: Repulsion and Dispersion. Journal of Chemical Theory and Computation, 2013, 9, 2264-2275.	5.3	64
17	Relation between exchange-only optimized potential and Kohnâ€“Sham methods with finite basis sets, and effect of linearly dependent products of orbital basis functions. Journal of Chemical Physics, 2008, 128, 104104.	3.0	61
18	Random-phase-approximation correlation method including exchange interactions. Physical Review A, 2012, 85, .	2.5	60

#	Article	IF	Citations
19	Resolution of identity approach for the Kohn-Sham correlation energy within the exact-exchange random-phase approximation. Journal of Chemical Physics, 2012, 136, 134102.	3.0	52
20	The coulombic Ïƒ-hole model describes bonding in CX₃Iâ‹¯Y^{â”} complexes completely. Physical Chemistry Chemical Physics, 2018, 20, 22849-22855.	2.8	50
21	Charge-transfer excitation energies with a time-dependent density-functional method suitable for orbital-dependent exchange-correlation kernels. Physical Review A, 2009, 80, .	2.5	49
22	Comparison of Intermolecular Interaction Energies from SAPT and DFT Including Empirical Dispersion Contributions. Journal of Physical Chemistry A, 2011, 115, 11321-11330.	2.5	48
23	Trifluoromethyl: An Amphiphilic Noncovalent Bonding Partner. ChemPhysChem, 2017, 18, 772-784.	2.1	47
24	Derivation of the dispersion energy as an explicit density- and exchange-hole functional. Journal of Chemical Physics, 2009, 130, 084104.	3.0	34
25	Comparison between optimized effective potential and Kohnâ€“Sham methods. Chemical Physics Letters, 2008, 455, 110-119.	2.6	30
26	First-order intermolecular interaction energies from coupled-cluster Brueckner orbitals. Journal of Chemical Physics, 2000, 112, 6949-6952.	3.0	28
27	The role of orbital transformations in coupled-pair functionals. Theoretical Chemistry Accounts, 2010, 127, 311-325.	1.4	28
28	Third-order corrections to random-phase approximation correlation energies. Journal of Chemical Physics, 2011, 134, 204107.	3.0	28
29	Assessment of a Nonlocal Correction Scheme to Semilocal Density Functional Theory Methods. Journal of Chemical Theory and Computation, 2013, 9, 273-283.	5.3	27
30	DFT-SAPT Intermolecular Interaction Energies Employing Exact-Exchange Kohnâ€“Sham Response Methods. Journal of Chemical Theory and Computation, 2018, 14, 1943-1959.	5.3	27
31	Efficient exact-exchange time-dependent density-functional theory methods and their relation to time-dependent Hartreeâ€“Fock. Journal of Chemical Physics, 2011, 134, 034120.	3.0	25
32	Molecular excitation spectra by TDDFT with the nonadiabatic exact exchange kernel. International Journal of Quantum Chemistry, 2010, 110, 2202-2220.	2.0	23
33	Molecular properties from coupled-cluster Brueckner orbitals. Chemical Physics Letters, 1999, 315, 248-256.	2.6	21
34	Molecular energies from an incremental fragmentation method. Journal of Chemical Physics, 2016, 144, 084109.	3.0	21
35	Accurate Intermolecular Potential for the C₆₀ Dimer: The Performance of Different Levels of Quantum Theory. Journal of Chemical Theory and Computation, 2017, 13, 274-285.	5.3	20
36	On the Short-Range Behavior of Correlated Pair Functions from the Adiabatic-Connection Fluctuationâ€“Dissipation Theorem of Density-Functional Theory. Journal of Chemical Theory and Computation, 2013, 9, 4382-4395.	5.3	17

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37	Intramolecular interactions in sterically crowded hydrocarbon molecules. Journal of Computational Chemistry, 2017, 38, 2500-2508.	3.3	17
38	Density-Functional Theory with Orbital-Dependent Functionals: Exact-exchange Kohn-Sham and Density-Functional Response Methods. Zeitschrift Fur Physikalische Chemie, 2010, 224, 325-342.	2.8	16
39	Long-range correlation energies from frequency-dependent weighted exchange-hole dipole polarisabilities. Journal of Chemical Physics, 2012, 136, 014104.	3.0	15
40	On the Stability of Cyclophane Derivates Using a Molecular Fragmentation Method. ChemPhysChem, 2016, 17, 3863-3874.	2.1	12
41	Molecular Excitation Energies from Time-Dependent Density Functional Theory Employing Random-Phase Approximation Hessians with Exact Exchange. Journal of Chemical Theory and Computation, 2015, 11, 1607-1620.	5.3	9
42	Comment on â€œPhysisorption of Water on Graphene: Subchemical Accuracy from Many-Body Electronic Structure Methodsâ€. Journal of Physical Chemistry C, 2019, 123, 10163-10165.	3.1	9
43	Polarisabilities of long conjugated chain molecules with density functional response methods: The role of coupled and uncoupled response. Journal of Chemical Physics, 2015, 142, 164102.	3.0	6
44	Assessment of a range-separated orbital-optimised random-phase approximation electron correlation method. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	6
45	Geometry optimizations with the incremental molecular fragmentation method. Journal of Theoretical and Computational Chemistry, 2018, 17, 1850037.	1.8	5
46	Study of the Wilcox torsion balance in solution for a TrÃ¶gerâ€™s base derivative with hexyl-and heptyl substituents using a combined molecular mechanics and quantum chemistry approach. Journal of Molecular Modeling, 2019, 25, 69.	1.8	4
47	The Feynman dispersion correction for MNDO extended to F, Cl, Br and I. Journal of Molecular Modeling, 2019, 25, 156.	1.8	3
48	Geometry optimisations with a nonlocal density-functional theory method based on a double Hirshfeld partitioning. Journal of Chemical Physics, 2018, 149, 044103.	3.0	2
49	Intermolecular interaction energies from fourth order many-body perturbation theory. Impact of individual electron correlation contributions. Journal of Chemical Physics, 2019, 151, 114105.	3.0	1
50	The Feynman dispersion correction for MNDO extended to F, Cl, Br and I. , 2019, 25, 1.		1