J Grant Hill

List of Publications by Year
in descending order

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61 papers	2,624 citations	257450 24 h-index	182427 51 g-index
65 all docs	65 docs citations	65 times ranked	2568 citing authors

#	Article	IF	Citations
1	Correlation consistent basis sets for molecular core-valence effects with explicitly correlated wave functions: The atoms Bâ€“Ne and Alâ€“Ar. Journal of Chemical Physics, 2010, 132, 054108.	3.0	253
2	Extrapolating MP2 and CCSD explicitly correlated correlation energies to the complete basis set limit with first and second row correlation consistent basis sets. Journal of Chemical Physics, 2009, 131, 194105.	3.0	251
3	On the effectiveness of CCSD(T) complete basis set extrapolations for atomization energies. Journal of Chemical Physics, 2011, 135, 044102.	3.0	250
4	Calculation of intermolecular interactions in the benzene dimer using coupled-cluster and local electron correlation methods. Physical Chemistry Chemical Physics, 2006, 8, 4072.	2.8	211
5	Gaussian basis sets for molecular applications. International Journal of Quantum Chemistry, 2013, 113, 21-34.	2.0	152
6	Gaussian basis sets for use in correlated molecular calculations. XI. Pseudopotential-based and all-electron relativistic basis sets for alkali metal (Kâ€“Fr) and alkaline earth (Caâ€“Ra) elements. Journal of Chemical Physics, 2017, 147, 244106.	3.0	144
7	Spin-Component Scaling Methods for Weak and Stacking Interactions. Journal of Chemical Theory and Computation, 2007, 3, 80-85.	5.3	136
8	Assessment of the Performance of MP2 and MP2 Variants for the Treatment of Noncovalent Interactions. Journal of Physical Chemistry A, 2012, 116, 4159-4169.	2.5	107
9	Correlation consistent basis sets for explicitly correlated wavefunctions: valence and coreâ€“valence basis sets for Li, Be, Na, and Mg. Physical Chemistry Chemical Physics, 2010, 12, 10460.	2.8	104
10	Explicitly correlated composite thermochemistry of transition metal species. Journal of Chemical Physics, 2013, 139, 094302.	3.0	79
11	Correlation consistent basis sets for explicitly correlated wavefunctions: Pseudopotential-based basis sets for the post-d main group elements Gaâ€“Rn. Journal of Chemical Physics, 2014, 141, 094106.	3.0	62
12	Calibration study of the CCSD(T)-F12a/b methods for C2 and small hydrocarbons. Journal of Chemical Physics, 2010, 133, 184102.	3.0	57
13	On the directionality and non-linearity of halogen and hydrogen bonds. Physical Chemistry Chemical Physics, 2015, 17, 858-867.	2.8	52
14	Experimental Electron Density and Neutron Diffraction Studies on the Polymorphs of Sulfathiazole. Crystal Growth and Design, 2014, 14, 1227-1239.	3.0	46
15	Calculating stacking interactions in nucleic acid base-pair steps using spin-component scaling and local second order MÃ¸llerâ€“Plesset perturbation theory. Physical Chemistry Chemical Physics, 2008, 10, 2785.	2.8	45
16	Auxiliary basis sets for density fittingâ€“MP2 calculations: Nonrelativistic triple-Î¶ all-electron correlation consistent basis sets for the 3d elements Scâ€“Zn. Journal of Chemical Physics, 2008, 128, 044104.	3.0	43
17	Explicitly Correlated Coupled Cluster Calculations for Molecules Containing Group 11 (Cu, Ag, Au) and 12 (Zn, Cd, Hg) Elements: Optimized Complementary Auxiliary Basis Sets for Valence and Coreâ€“Valence Basis Sets. Journal of Chemical Theory and Computation, 2012, 8, 518-526.	5.3	39
18	Theoretical Insights into the Nature of Halogen Bonding in Prereactive Complexes. Chemistry - A European Journal, 2013, 19, 3620-3628.	3.3	39

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19	Insights into DNA Binding of Ruthenium Arene Complexes: Role of Hydrogen Bonding and Ï€ Stacking. Inorganic Chemistry, 2008, 47, 3893-3902.	4.0	36
20	Application of explicitly correlated coupled-cluster methods to molecules containing post-3d main group elements. Molecular Physics, 2011, 109, 2607-2623.	1.7	33
21	Halogen Bonding with Phosphine: Evidence for Mulliken Inner Complexes and the Importance of Relaxation Energy. Journal of Physical Chemistry A, 2016, 120, 8461-8468.	2.5	30
22	Accurate ab initio ro-vibronic spectroscopy of the $ilde X^2 Pi$XÌƒ2Î CCN radical using explicitly correlated methods. Journal of Chemical Physics, 2011, 135, 144309.	3.0	29
23	Auxiliary Basis Sets for Density Fitting in Explicitly Correlated Calculations: The Atoms Hâ€“Ar. Journal of Chemical Theory and Computation, 2015, 11, 5269-5276.	5.3	29
24	Ab initio ro-vibrational spectroscopy of the group 11 cyanides: CuCN, AgCN, and AuCN. Journal of Chemical Physics, 2013, 138, 134314.	3.0	25
25	Local electron correlation descriptions of the intermolecular stacking interactions between aromatic intercalators and nucleic acids. Chemical Physics Letters, 2009, 479, 279-283.	2.6	24
26	The halogen bond in thiiraneâ‹¯ClF: an example of a Mulliken inner complex. Physical Chemistry Chemical Physics, 2014, 16, 19137.	2.8	22
27	Approaching the Hartreeâ€“Fock Limit through the Complementary Auxiliary Basis Set Singles Correction and Auxiliary Basis Sets. Journal of Chemical Theory and Computation, 2017, 13, 1691-1698.	5.3	21
28	Auxiliary basis sets for density fitting second-order MÃ¸ller-Plesset perturbation theory: Correlation consistent basis sets for the 5d elements Hf-Pt. Journal of Chemical Physics, 2011, 135, 044105.	3.0	20
29	Near-UV photodissociation dynamics of CH₂I₂. Physical Chemistry Chemical Physics, 2016, 18, 11091-11103.	2.8	19
30	A spin-coupled study of the Claisen rearrangement of allyl vinyl ether. Theoretical Chemistry Accounts, 2006, 115, 212-220.	1.4	18
31	Structures and Heats of Formation of Simple Alkaline Earth Metal Compounds II: Fluorides, Chlorides, Oxides, and Hydroxides for Ba, Sr, and Ra. Journal of Physical Chemistry A, 2018, 122, 316-327.	2.5	18
32	Performance of Beckeâ€™s half-and-half functional for non-covalent interactions: energetics, geometries and electron densities. Journal of Molecular Modeling, 2009, 15, 1051-1060.	1.8	17
33	Auxiliary Basis Sets for Density-Fitted MP2 Calculations: Correlation-Consistent Basis Sets for the 4d Elements. Journal of Chemical Theory and Computation, 2009, 5, 500-505.	5.3	17
34	Calculating interaction energies in transition metal complexes with local electron correlation methods. Journal of Chemical Physics, 2008, 129, 134101.	3.0	14
35	Interplay between hydrogen bonding and nâ†’Ï€* interaction in an analgesic drug salicin. Physical Chemistry Chemical Physics, 2018, 20, 18361-18373.	2.8	14
36	Basis Set Dependence of Interaction Energies Computed Using Composite Post-MP2 Methods. Journal of Chemical Theory and Computation, 2013, 9, 330-337.	5.3	12

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37	Midbond basis functions for weakly bound complexes. Molecular Physics, 2018, 116, 1460-1470.	1.7	12
38	A Simple Model for Halogen Bond Interaction Energies. Inorganics, 2019, 7, 19.	2.7	11
39	The unusual electronic mechanism of the [1,5] hydrogen shift in (Z)-1,3-pentadiene predicted by modern valence bond theory. Faraday Discussions, 2007, 135, 285-297.	3.2	10
40	Spin-Coupled Description of Aromaticity in the Retro Dielsâ^'Alder Reaction of Norbornene. Journal of Physical Chemistry A, 2008, 112, 12823-12828.	2.5	9
41	Auxiliary basis sets for density-fitting second-order MÃ¸ller-Plesset perturbation theory: Weighted core-valence correlation consistent basis sets for the 4delements Y-Pd. Journal of Computational Chemistry, 2013, 34, 2168-2177.	3.3	9
42	An ab initio investigation of alkaliâ€“metal non-covalent bonds Bâ‹¯LiR and Bâ‹¯NaR (R = F, H or) Tj ETQq0 0 0 rgBT /Overlock 10 T CH₃. Physical Chemistry Chemical Physics, 2020, 22, 16421-16430.	2.8	9
43	Alkali-Metal Trihalides: M+X3â€“Ion Pair or MXâ€“X2Complex?. Journal of Physical Chemistry B, 2018, 122, 3339-3353.	2.6	8
44	Syntheses, Structures, and Infrared Spectra of the Hexa(cyanido) Complexes of Silicon, Germanium, and Tin. Inorganic Chemistry, 2019, 58, 4583-4591.	4.0	8
45	Modern Valence-Bond-Like Representations of SelectedD6hâ€œAromaticâ€•Rings. Journal of Physical Chemistry A, 2006, 110, 7913-7917.	2.5	7
46	Halogen Bonding in the Gas Phase: A Comparison of the Iodine Bond in Bâ‹¯ICl and Bâ‹¯ICF3 for Simple Lewis Bases B. Topics in Current Chemistry, 2014, 358, 43-77.	4.0	7
47	(Ï€*,Ïƒ*), (Ïƒ*,Ï€*) and Rydberg Triplet Excited States of Hydrogen Peroxide and Other Molecules Bearing Two Adjacent Heteroatoms. Journal of Physical Chemistry A, 2014, 118, 2332-2343.	2.5	7
48	Interplay among Electrostatic, Dispersion, and Steric Interactions: Spectroscopy and Quantum Chemical Calculations of Ï€â€Hydrogen Bonded Complexes. ChemPhysChem, 2017, 18, 828-838.	2.1	7
49	The spin-coupled picture of clamped benzenes. Molecular Physics, 2006, 104, 677-680.	1.7	6
50	Prescreening and efficiency in the evaluation of integrals over ab initio effective core potentials. Journal of Chemical Physics, 2017, 147, 074108.	3.0	6
51	CHARMM-DYES: Parameterization of Fluorescent Dyes for Use with the CHARMM Force Field. Journal of Chemical Theory and Computation, 2020, 16, 7817-7824.	5.3	6
52	Non-covalent interactions using local correlation methods: energy partitioning, geometry optimisation and harmonic frequency calculations. Molecular Physics, 2010, 108, 1497-1504.	1.7	5
53	Interaction in the indoleâ‹¯imidazole heterodimer: structure, Franckâ€“Condon analysis and energy decomposition. Physical Chemistry Chemical Physics, 2014, 16, 11754.	2.8	5
54	Correlation consistent basis sets for explicitly correlated wavefunctions: Pseudopotential-based basis sets for the group 11 (Cu, Ag, Au) and 12 (Zn, Cd, Hg) elements. Journal of Chemical Physics, 2021, 155, 174113.	3.0	5

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55	A Linear-Scaling Method for Noncovalent Interactions: An Efficient Combination of Absolutely Localized Molecular Orbitals and a Local Random Phase Approximation Approach. Journal of Chemical Theory and Computation, 2019, 15, 5352-5369.	5.3	4
56	Optimized Basis Sets for the Environment in the Domain-Specific Basis Set Approach of the Incremental Scheme. Journal of Physical Chemistry A, 2016, 120, 2443-2458.	2.5	3
57	UV photodissociation dynamics of CHI2Cl and its role as a photolytic precursor for a chlorinated Criegee intermediate. Physical Chemistry Chemical Physics, 2017, 19, 31039-31053.	2.8	3
58	libecpint: A C++ library for the efficient evaluation of integrals over effective core potentials. Journal of Open Source Software, 2021, 6, 3039.	4.6	3
59	Nonbonding pairs in cyclic thioethers: Electrostatic modeling and ab initio calculations for complexes of 2,5â€dihydrothiophene, thietane, and thiirane with hydrogen fluoride. International Journal of Quantum Chemistry, 2019, 119, e25885.	2.0	2
60	Radial Potential Energy Functions of Linear Halogen-Bonded Complexes YXÂ·Â·Â·ClF (YX = FB, OC, SC,) Tj ETQq0 0 0 rgBT /Overlock 10 T Complexes. Journal of Physical Chemistry A, 2022, , .	2.5	2
61	Electrostatic Potential and a Simple Extended Electric Dipole Model of Hydrogen Fluoride as Probes of Non-Bonding Electron Pairs in the Cyclic Ethers 2,5-Dihydrofuran, Oxetane and Oxirane. Crystals, 2017, 7, 261.	2.2	1