Edward F Valeev

List of Publications by Citations

106 papers	9,101 citations	39 h-index	95 g-index
112 ext. papers	10,112 ext. citations	5.6 avg, IF	6.3 L-index

#	Paper	IF	Citations
106	Estimates of the ab initio limit for pi-pi interactions: the benzene dimer. *Journal of the American Chemical Society*, **2002**, 124, 10887-93	16.4	1112
105	Psi4 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability. *Journal of Chemical Theory and Computation*, **2017**, 13, 3185-3197	6.4	733
104	Psi4: an open-source ab initio electronic structure program. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 556-565	7.9	678
103	Effect of electronic polarization on charge-transport parameters in molecular organic semiconductors. *Journal of the American Chemical Society*, **2006**, 128, 9882-6	16.4	652
102	HEAT: High accuracy extrapolated ab initio thermochemistry. *Journal of Chemical Physics*, **2004**, 121, 11599-613	3.9	606
101	Sparse maps--A systematic infrastructure for reduced-scaling electronic structure methods. II. Linear scaling domain based pair natural orbital coupled cluster theory. *Journal of Chemical Physics*, **2016**, 144, 024109	3.9	489
100	R12 methods in explicitly correlated molecular electronic structure theory. *International Reviews in Physical Chemistry*, **2006**, 25, 427-468	7	360
99	Explicitly correlated R12/F12 methods for electronic structure. *Chemical Reviews*, **2012**, 112, 75-107	68.1	334
98	Improving on the resolution of the identity in linear R12 ab initio theories. *Chemical Physics Letters*, **2004**, 395, 190-195	2.5	318
97	PSI3: an open-source Ab Initio electronic structure package. *Journal of Computational Chemistry*, **2007**, 28, 1610-1616	3.5	249
96	Anchoring the water dimer potential energy surface with explicitly correlated computations and focal point analyses. *Journal of Chemical Physics*, **2002**, 116, 690-701	3.9	239
95	Revisiting the Atomic Natural Orbital Approach for Basis Sets: Robust Systematic Basis Sets for Explicitly Correlated and Conventional Correlated ab initio Methods?. *Journal of Chemical Theory and Computation*, **2011**, 7, 33-43	6.4	195
94	A new near-linear scaling, efficient and accurate, open-shell domain-based local pair natural orbital coupled cluster singles and doubles theory. *Journal of Chemical Physics*, **2017**, 146, 164105	3.9	194
93	Sparse maps—A systematic infrastructure for reduced-scaling electronic structure methods. I. An efficient and simple linear scaling local MP2 method that uses an intermediate basis of pair natural orbitals. *Journal of Chemical Physics*, **2015**, 143, 034108	3.9	169
92	Analysis of the errors in explicitly correlated electronic structure theory. *Physical Chemistry Chemical Physics*, **2005**, 7, 2710-3	3.6	113
91	The diagonal Born–Oppenheimer correction beyond the Hartree–Fock approximation. *Journal of Chemical Physics*, **2003**, 118, 3921-3927	3.9	113
90	CVRQD ab initio ground-state adiabatic potential energy surfaces for the water molecule. *Journal of Chemical Physics*, **2006**, 125, 204307	3.9	106

89	SparseMaps--A systematic infrastructure for reduced-scaling electronic structure methods. III. Linear-scaling multireference domain-based pair natural orbital N-electron valence perturbation theory. *Journal of Chemical Physics*, **2016**, 144, 094111	3.9	105
88	Simple coupled-cluster singles and doubles method with perturbative inclusion of triples and explicitly correlated geminals: The CCSD(T)R12 model. *Journal of Chemical Physics*, **2008**, 128, 244113	3.9	99
87	The protonated water dimer: Brueckner methods remove the spurious C1 symmetry minimum. *Journal of Chemical Physics*, **1998**, 108, 7197-7201	3.9	98
86	Coupled-cluster methods with perturbative inclusion of explicitly correlated terms: a preliminary investigation. *Physical Chemistry Chemical Physics*, **2008**, 10, 106-13	3.6	94
85	Explicitly correlated coupled-cluster singles and doubles method based on complete diagrammatic equations. *Journal of Chemical Physics*, **2008**, 129, 071101	3.9	87
84	SparseMaps-A systematic infrastructure for reduced scaling electronic structure methods. V. Linear scaling explicitly correlated coupled-cluster method with pair natural orbitals. *Journal of Chemical Physics*, **2017**, 146, 174108	3.9	84
83	Variational formulation of perturbative explicitly-correlated coupled-cluster methods. *Physical Chemistry Chemical Physics*, **2008**, 10, 3410-20	3.6	77
82	SparseMaps--A systematic infrastructure for reduced-scaling electronic structure methods. IV. Linear-scaling second-order explicitly correlated energy with pair natural orbitals. *Journal of Chemical Physics*, **2016**, 144, 144109	3.9	77
81	The electron and nuclear orbitals model: current challenges and future prospects. *Molecular Physics* , **2004**, 102, 111-123	1.7	72
80	Higher-order explicitly correlated coupled-cluster methods. *Journal of Chemical Physics*, **2009**, 130, 054104	3.9	71
79	Equations of explicitly-correlated coupled-cluster methods. *Physical Chemistry Chemical Physics*, **2008**, 10, 3358-70	3.6	70
78	On the accuracy limits of orbital expansion methods: Explicit effects of k-functions on atomic and molecular energies. *Journal of Chemical Physics*, **2003**, 118, 8594-8610	3.9	68
77	Second-order Møller-Plesset theory with linear R12 terms (MP2-R12) revisited: auxiliary basis set method and massively parallel implementation. *Journal of Chemical Physics*, **2004**, 121, 1214-27	3.9	64
76	Universal perturbative explicitly correlated basis set incompleteness correction. *Journal of Chemical Physics*, **2009**, 131, 171103	3.9	63
75	Combining explicitly correlated R12 and Gaussian geminal electronic structure theories. *Journal of Chemical Physics*, **2006**, 125, 244106	3.9	59
74	Adaptive Steered Molecular Dynamics of the Long-Distance Unfolding of Neuropeptide Y. *Journal of Chemical Theory and Computation*, **2010**, 6, 3026-38	6.4	58
73	Prediction of Reaction Barriers and Thermochemical Properties with Explicitly Correlated Coupled-Cluster Methods: A Basis Set Assessment. *Journal of Chemical Theory and Computation*, **2012**, 8, 3175-86	6.4	56
72	MADNESS: A Multiresolution, Adaptive Numerical Environment for Scientific Simulation. *SIAM Journal of Scientific Computing*, **2016**, 38, S123-S142	2.6	48

71	The second-order Møller-Plesset limit for the barrier to linearity of water. *Journal of Chemical Physics*, **2001**, 114, 2875-2878	3.9	47
70	Evaluation of two-electron integrals for explicit r12 theories. *Journal of Chemical Physics*, **2000**, 113, 3990-3995	3.9	43
69	Comparison of one-particle basis set extrapolation to explicitly correlated methods for the calculation of accurate quartic force fields, vibrational frequencies, and spectroscopic constants: application to H2O, N2H+, NO2+, and C2H2. *Journal of Chemical Physics*, **2010**, 133, 244108	3.9	42
68	Massively Parallel Implementation of Explicitly Correlated Coupled-Cluster Singles and Doubles Using TiledArray Framework. *Journal of Physical Chemistry A*, **2016**, 120, 10231-10244	2.8	39
67	Low-order tensor approximations for electronic wave functions: Hartree-Fock method with guaranteed precision. *Journal of Chemical Physics*, **2011**, 134, 104104	3.9	35
66	Computing many-body wave functions with guaranteed precision: the first-order Møller-Plesset wave function for the ground state of helium atom. *Journal of Chemical Physics*, **2012**, 137, 104103	3.9	34
65	Geminal-spanning orbitals make explicitly correlated reduced-scaling coupled-cluster methods robust, yet simple. *Journal of Chemical Physics*, **2014**, 141, 054106	3.9	33
64	Explicitly correlated combined coupled-cluster and perturbation methods. *Journal of Chemical Physics*, **2009**, 131, 044118	3.9	33
63	The Chronus Quantum software package. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2020**, 10, e1436	7.9	31
62	What is the most efficient way to reach the canonical MP2 basis set limit?. *Molecular Physics*, **2013**, 111, 2653-2662	1.7	30
61	Semi-exact concentric atomic density fitting: reduced cost and increased accuracy compared to standard density fitting. *Journal of Chemical Physics*, **2014**, 140, 064109	3.9	29
60	Computing molecular correlation energies with guaranteed precision. *Journal of Chemical Physics*, **2013**, 139, 114106	3.9	29
59	Perturbative correction for the basis set incompleteness error of complete-active-space self-consistent field. *Journal of Chemical Physics*, **2010**, 133, 174126	3.9	29
58	A Comparison of One-Particle Basis Set Completeness, Higher-Order Electron Correlation, Relativistic Effects, and Adiabatic Corrections for Spectroscopic Constants of BH, CH+, and NH *Journal of Physical Chemistry A*, **2004**, 108, 3068-3075	2.8	28
57	Coupled-cluster singles, doubles and perturbative triples with density fitting approximation for massively parallel heterogeneous platforms. *International Journal of Quantum Chemistry*, **2019**, 119, e25894	2.1	28
56	Efficient implementation of the analytic second derivatives of Hartree–Fock and hybrid DFT energies: a detailed analysis of different approximations. *Molecular Physics*, **2015**, 113, 1961-1977	1.7	27
55	SF-[2]R12: a spin-adapted explicitly correlated method applicable to arbitrary electronic states. *Journal of Chemical Physics*, **2011**, 135, 214105	3.9	26
54	Three- versus four-coordinate phosphorus in the gas phase and in solution: Treacherous relative energies for phosphine oxide and phosphinous acid. *Journal of Chemical Physics*, **2002**, 116, 112	3.9	25

53	Chapter 6 Explicitly Correlated Coupled-Cluster Methods. *Annual Reports in Computational Chemistry*, **2009**, 131-148	1.8	24
52	State-Averaged Pair Natural Orbitals for Excited States: A Route toward Efficient Equation of Motion Coupled-Cluster. *Journal of Chemical Theory and Computation*, **2018**, 14, 5597-5607	6.4	24
51	(1,2-Diaminoethane-1,2-diyl)bis(N-methylpyridinium) Salts as a Prospective Platform for Designing Recyclable Prolinamide-Based Organocatalysts. *Journal of Organic Chemistry*, **2015**, 80, 9570-7	4.2	22
50	A novel interpretation of reduced density matrix and cumulant for electronic structure theories. *Journal of Chemical Physics*, **2011**, 134, 214109	3.9	22
49	C60complexes with dianthracene and triptycene: synthesis and crystal structures. *Synthetic Metals*, **1999**, 103, 2364-2365	3.6	22
48	Is the adiabatic approximation sufficient to account for the post-Born□Oppenheimer effects on molecular electric dipole moments?. *Molecular Physics*, **2009**, 107, 1153-1159	1.7	18
47	Communication: stochastic evaluation of explicitly correlated second-order many-body perturbation energy. *Journal of Chemical Physics*, **2014**, 140, 031101	3.9	17
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44	Clustered Low-Rank Tensor Format: Introduction and Application to Fast Construction of Hartree-Fock Exchange. *Journal of Chemical Theory and Computation*, **2016**, 12, 5868-5880	6.4	17
43	A tight distance-dependent estimator for screening three-center Coulomb integrals over Gaussian basis functions. *Journal of Chemical Physics*, **2015**, 142, 154106	3.9	16
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41	Interlocking Triplet Electronic States of Isocyanic Acid: Sources of Nonadiabatic Photofragmentation Dynamics□*Journal of Physical Chemistry A*, **2001**, 105, 2716-2730	2.8	14
40	Explicitly correlated N-electron valence state perturbation theory (NEVPT2-F12). *Journal of Chemical Physics*, **2017**, 147, 064110	3.9	13
39	Computation of precise two-electron correlation energies with imprecise Hartree□ock orbitals. *Chemical Physics Letters*, **2006**, 418, 333-336	2.5	13
38	Communication: Explicitly correlated formalism for second-order single-particle Green□s function. *Journal of Chemical Physics*, **2017**, 147, 121101	3.9	12
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36	Massively Parallel Quantum Chemistry: A high-performance research platform for electronic structure. *Journal of Chemical Physics*, **2020**, 153, 044120	3.9	12

35	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. *Chemical Reviews*, **2021**, 121, 4962-4998	68.1	12
34	Monte Carlo explicitly correlated second-order many-body perturbation theory. *Journal of Chemical Physics*, **2016**, 145, 154115	3.9	12
33	Optimized Pair Natural Orbitals for the Coupled Cluster Methods. *Journal of Chemical Theory and Computation*, **2018**, 14, 4581-4589	6.4	11
32	A New Class of Supramolecular Wires. *Journal of Physical Chemistry C*, **2007**, 111, 18912-18916	3.8	11
31	Quantum simulation of electronic structure with a transcorrelated Hamiltonian: improved accuracy with a smaller footprint on the quantum computer. *Physical Chemistry Chemical Physics*, **2020**, 22, 24270-24281	3.6	11
30	A series of new molecular complexes C60(S4N4)2 □x(C6H6)x: Synthesis, x-ray study of crystal structure and structural disorder. *Journal of Physics and Chemistry of Solids*, **1997**, 58, 1865-1867	3.9	10
29	The not-so-peculiar case of calcium oxide: a weakness in atomic natural orbital basis sets for calcium. *Molecular Physics*, **2000**, 98, 1227-1231	1.7	10
28	Explicitly correlated second-order M□ller-Plesset perturbation theory in a Divide-Expand-Consolidate (DEC) context. *Journal of Chemical Physics*, **2016**, 144, 204112	3.9	10
27	Scalable task-based algorithm for multiplication of block-rank-sparse matrices **2015**,		9
26	Assessment of Perturbative Explicitly Correlated Methods for Prototypes of Multiconfiguration Electronic Structure. *Journal of Chemical Theory and Computation*, **2014**, 10, 90-101	6.4	8
25	The elementary reaction of quartet methylidyne (CH) with methane. *Molecular Physics*, **1996**, 89, 1695-1705	1.7	8
24	Can the distinguishable cluster approximation be improved systematically by including connected triples?. *Journal of Chemical Physics*, **2019**, 151, 064102	3.9	7
23	. *Computing in Science and Engineering*, **2019**, 21, 48-58	1.5	7
22	Explicitly correlated renormalized second-order Green□s function for accurate ionization potentials of closed-shell molecules. *Journal of Chemical Physics*, **2019**, 150, 214103	3.9	6
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20	EXAFS study of the M0.5(OH)x(H2O)yMoS2 intercalated complexes. *Physica B: Condensed Matter*, **1995**, 208-209, 569-570	2.8	6
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17	Fast construction of the exchange operator in an atom-centred basis with concentric atomic density fitting. *Molecular Physics*, **2017**, 115, 2065-2076	1.7	5
16	Anatomy of molecular properties evaluated with explicitly correlated electronic wave functions. *Molecular Physics*, **2016**, 114, 2894-2909	1.7	5
15	Effective Utilization of Tensor Symmetry in Operation Optimization of Tensor Contraction Expressions. *Procedia Computer Science*, **2012**, 9, 412-421	1.6	4
14	Chapter 2 Explicitly Correlated Approaches for Electronic Structure Computations. *Annual Reports in Computational Chemistry*, **2006**, 2, 19-33	1.8	4
13	Explicitly correlated coupled cluster method for accurate treatment of open-shell molecules with hundreds of atoms. *Journal of Chemical Physics*, **2020**, 153, 094105	3.9	4
12	Efficient Four-Component Dirac-Coulomb-Gaunt Hartree-Fock in the Pauli Spinor Representation. *Journal of Chemical Theory and Computation*, **2021**, 17, 3388-3402	6.4	4
11	Robust Approximation of Tensor Networks: Application to Grid-Free Tensor Factorization of the Coulomb Interaction. *Journal of Chemical Theory and Computation*, **2021**, 17, 2217-2230	6.4	4
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9	Efficient evaluation of exact exchange for periodic systems via concentric atomic density fitting. *Journal of Chemical Physics*, **2020**, 153, 124116	3.9	3
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7	Combined Relativistic Ab Initio Multireference and Experimental Study of the Electronic Structure of Terbium Luminescent Compound. *Journal of Physical Chemistry A*, **2020**, 124, 82-89	2.8	2
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1	Eclectic Electron-Correlation Methods. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 191-217	0.7	