Edward F Valeev

List of Publications by Year
in descending order

112 papers	11,063 citations	71102 41 h-index	30087 103 g-index
113 all docs	113 docs citations	113 times ranked	8494 citing authors

#	Article	IF	Citations
1	Generalized Flow-Graph Programming Using Template Task-Graphs: Initial Implementation and Assessment. , 2022, , .		2
2	Many-Body Quantum Chemistry on Massively Parallel Computers. Chemical Reviews, 2021, 121, 1203-1231.	47.7	21
3	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.	5.3	8
4	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998.	47.7	39
5	Toward the Minimal Floating Operation Count Cholesky Decomposition of Electron Repulsion Integrals. Journal of Physical Chemistry A, 2021, 125, 4258-4265.	2.5	11
6	Distributed-memory multi-GPU block-sparse tensor contraction for electronic structure. , 2021, , .		4
7	Efficient Four-Component Diracâ€“Coulombâ€“Gaunt Hartreeâ€“Fock in the Pauli Spinor Representation. Journal of Chemical Theory and Computation, 2021, 17, 3388-3402.	5.3	24
8	Robust Pipekâ€“Mezey Orbital Localization in Periodic Solids. Journal of Chemical Theory and Computation, 2021, 17, 7406-7415.	5.3	2
9	The Chronus Quantum software package. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1436.	14.6	66
10	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.	2.5	5
11	Massively Parallel Quantum Chemistry: A high-performance research platform for electronic structure. Journal of Chemical Physics, 2020, 153, 044120.	3.0	25
12	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.	2.8	43
13	Explicitly correlated coupled cluster method for accurate treatment of open-shell molecules with hundreds of atoms. Journal of Chemical Physics, 2020, 153, 094105.	3.0	22
14	Efficient evaluation of exact exchange for periodic systems via concentric atomic density fitting. Journal of Chemical Physics, 2020, 153, 124116.	3.0	12
15	Comment on â€œA tight distance-dependent estimator for screening three-center Coulomb integrals over Gaussian basis functionsâ€•[J. Chem. Phys. 142, 154106 (2015)]. Journal of Chemical Physics, 2020, 153, 097101.	3.0	2
16	Direct determination of optimal pair-natural orbitals in a real-space representation: The second-order Mollerâ€“Plesset energy. Journal of Chemical Physics, 2020, 152, 074105.	3.0	15
17	The Template Task Graph (TTG) - an emerging practical dataflow programming paradigm for scientific simulation at extreme scale. , 2020, , .		6
18	Explicitly correlated renormalized second-order Greenâ€™s function for accurate ionization potentials of closed-shell molecules. Journal of Chemical Physics, 2019, 150, 214103.	3.0	6

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19	Can the distinguishable cluster approximation be improved systematically by including connected triples?. Journal of Chemical Physics, 2019, 151, .	3.0	13
20	Developing a Computational Chemistry Framework for the Exascale Era. Computing in Science and Engineering, 2019, 21, 48-58.	1.2	16
21	Coupledâ€cluster singles, doubles and perturbative triples with density fitting approximation for massively parallel heterogeneous platforms. International Journal of Quantum Chemistry, 2019, 119, e25894.	2.0	37
22	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.	5.3	32
23	Optimized Pair Natural Orbitals for the Coupled Cluster Methods. Journal of Chemical Theory and Computation, 2018, 14, 4581-4589.	5.3	13
24	SparseMapsâ€"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.	3.0	122
25	<scp>Psi4</scp> 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability. Journal of Chemical Theory and Computation, 2017, 13, 3185-3197.	5.3	961
26	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.	3.0	285
27	Communication: Explicitly correlated formalism for second-order single-particle Greenâ€™s function. Journal of Chemical Physics, 2017, 147, 121101.	3.0	13
28	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
29	Explicitly correlated N-electron valence state perturbation theory (NEVPT2-F12). Journal of Chemical Physics, 2017, 147, 064110.	3.0	20
30	Anatomy of molecular properties evaluated with explicitly correlated electronic wave functions. Molecular Physics, 2016, 114, 2894-2909.	1.7	6
31	Clustered Low-Rank Tensor Format: Introduction and Application to Fast Construction of Hartreeâ€“Fock Exchange. Journal of Chemical Theory and Computation, 2016, 12, 5868-5880.	5.3	20
32	SparseMapsâ€"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.	3.0	131
33	SparseMapsâ€"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.	3.0	98
34	Explicitly correlated second-order MÃ¸ller-Plesset perturbation theory in a Divide-Expand-Consolidate (DEC) context. Journal of Chemical Physics, 2016, 144, 204112.	3.0	15
35	Massively Parallel Implementation of Explicitly Correlated Coupled-Cluster Singles and Doubles Using TiledArray Framework. Journal of Physical Chemistry A, 2016, 120, 10231-10244.	2.5	50
36	Sparse mapsâ€"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.	3.0	740

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37	Monte Carlo explicitly correlated second-order many-body perturbation theory. Journal of Chemical Physics, 2016, 145, 154115.	3.0	13
38	MADNESS: A Multiresolution, Adaptive Numerical Environment for Scientific Simulation. SIAM Journal of Scientific Computing, 2016, 38, S123-S142.	2.8	72
39	Spin-Free [2]_{R12} Basis Set Incompleteness Correction to the Local Multireference Configuration Interaction and the Local Multireference Average Coupled Pair Functional Methods. Journal of Chemical Theory and Computation, 2016, 12, 3176-3184.	5.3	3
40	Sparse mapsâ€"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.	3.0	211
41	Scalable task-based algorithm for multiplication of block-rank-sparse matrices. , 2015, , .		18
42	Efficient implementation of the analytic second derivatives of Hartreeâ€"Fock and hybrid DFT energies: a detailed analysis of different approximations. Molecular Physics, 2015, 113, 1961-1977.	1.7	38
43	A tight distance-dependent estimator for screening three-center Coulomb integrals over Gaussian basis functions. Journal of Chemical Physics, 2015, 142, 154106.	3.0	18
44	(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, 9570-9577.	3.2	26
45	Communication: Stochastic evaluation of explicitly correlated second-order many-body perturbation energy. Journal of Chemical Physics, 2014, 140, 031101.	3.0	18
46	Molecular Resonance Raman and Rayleigh Scattering Stimulated by a Short Laser Pulse. Journal of Statistical Physics, 2014, 154, 522-542.	1.2	1
47	Assessment of Perturbative Explicitly Correlated Methods for Prototypes of Multiconfiguration Electronic Structure. Journal of Chemical Theory and Computation, 2014, 10, 90-101.	5.3	10
48	Geminal-spanning orbitals make explicitly correlated reduced-scaling coupled-cluster methods robust, yet simple. Journal of Chemical Physics, 2014, 141, 054106.	3.0	36
49	Semi-exact concentric atomic density fitting: Reduced cost and increased accuracy compared to standard density fitting. Journal of Chemical Physics, 2014, 140, 064109.	3.0	33
50	Computing molecular correlation energies with guaranteed precision. Journal of Chemical Physics, 2013, 139, 114106.	3.0	31
51	What is the most efficient way to reach the canonical MP2 basis set limit?. Molecular Physics, 2013, 111, 2653-2662.	1.7	33
52	Explicitly Correlated R12/F12 Methods for Electronic Structure. Chemical Reviews, 2012, 112, 75-107.	47.7	408
53	Effective Utilization of Tensor Symmetry in Operation Optimization of Tensor Contraction Expressions. Procedia Computer Science, 2012, 9, 412-421.	2.0	7
54	Hybrid one-electron/many-electron methods for ionized states of molecular clusters. Physical Chemistry Chemical Physics, 2012, 14, 7863.	2.8	3

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55	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, 3175-3186.	5.3	79
56	Computing many-body wave functions with guaranteed precision: The first-order MÃ¸ller-Plesset wave function for the ground state of helium atom. Journal of Chemical Physics, 2012, 137, 104103.	3.0	40
57	Psi4: an openâ€source ab initio electronic structure program. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 556-565.	14.6	838
58	A novel interpretation of reduced density matrix and cumulant for electronic structure theories. Journal of Chemical Physics, 2011, 134, 214109.	3.0	24
59	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.	5.3	274
60	Low-order tensor approximations for electronic wave functions: Hartreeâ€“Fock method with guaranteed precision. Journal of Chemical Physics, 2011, 134, 104104.	3.0	42
61	$hbox{SF-[2]}_{ext{R12}}$ SF-[2] R12 : A spin-adapted explicitly correlated method applicable to arbitrary electronic states. Journal of Chemical Physics, 2011, 135, 214105.	3.0	29
62	Scalar relativistic explicitly correlated R12 methods. Journal of Chemical Physics, 2010, 132, 214104.	3.0	20
63	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.	3.0	55
64	Adaptive Steered Molecular Dynamics of the Long-Distance Unfolding of Neuropeptide Y. Journal of Chemical Theory and Computation, 2010, 6, 3026-3038.	5.3	88
65	Perturbative correction for the basis set incompleteness error of complete-active-space self-consistent field. Journal of Chemical Physics, 2010, 133, 174126.	3.0	30
66	Computational Interstellar Chemistry. Thirty Years of Astronomical Discovery With UKIRT, 2010, , 21-30.	0.3	0
67	Eclectic Electron-Correlation Methods. Challenges and Advances in Computational Chemistry and Physics, 2010, , 191-217.	0.6	0
68	Higher-order explicitly correlated coupled-cluster methods. Journal of Chemical Physics, 2009, 130, 054101.	3.0	73
69	Chapter 6 Explicitly Correlated Coupled-Cluster Methods. Annual Reports in Computational Chemistry, 2009, , 131-148.	1.7	24
70	Explicitly correlated combined coupled-cluster and perturbation methods. Journal of Chemical Physics, 2009, 131, 044118.	3.0	33
71	Is the adiabatic approximation sufficient to account for the post-Bornâ€“Oppenheimer effects on molecular electric dipole moments?. Molecular Physics, 2009, 107, 1153-1159.	1.7	20
72	Universal perturbative explicitly correlated basis set incompleteness correction. Journal of Chemical Physics, 2009, 131, 171103.	3.0	70

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73	Components for integral evaluation in quantum chemistry. Journal of Computational Chemistry, 2008, 29, 562-577.	3.3	21
74	Equations of explicitly-correlated coupled-cluster methods. Physical Chemistry Chemical Physics, 2008, 10, 3358.	2.8	77
75	Explicitly correlated coupled-cluster singles and doubles method based on complete diagrammatic equations. Journal of Chemical Physics, 2008, 129, 071101.	3.0	94
76	Simple coupled-cluster singles and doubles method with perturbative inclusion of triples and explicitly correlated geminals: The CCSD(T)R12Â¯ model. Journal of Chemical Physics, 2008, 128, 244113.	3.0	113
77	Variational formulation of perturbative explicitly-correlated coupled-cluster methods. Physical Chemistry Chemical Physics, 2008, 10, 3410.	2.8	85
78	Coupled-cluster methods with perturbative inclusion of explicitly correlated terms: a preliminary investigation. Physical Chemistry Chemical Physics, 2008, 10, 106-113.	2.8	106
79	PSI3: An open-source Ab Initio electronic structure package. Journal of Computational Chemistry, 2007, 28, 1610-1616.	3.3	258
80	A New Class of Supramolecular Wires. Journal of Physical Chemistry C, 2007, 111, 18912-18916.	3.1	12
81	Combining explicitly correlated R12 and Gaussian geminal electronic structure theories. Journal of Chemical Physics, 2006, 125, 244106.	3.0	59
82	Effect of Electronic Polarization on Charge-Transport Parameters in Molecular Organic Semiconductors. Journal of the American Chemical Society, 2006, 128, 9882-9886.	13.7	756
83	R12 methods in explicitly correlated molecular electronic structure theory. International Reviews in Physical Chemistry, 2006, 25, 427-468.	2.3	384
84	Enabling new capabilities and insights from quantum chemistry by using component architectures. Journal of Physics: Conference Series, 2006, 46, 220-228.	0.4	12
85	Computation of precise two-electron correlation energies with imprecise Hartreeâ€“Fock orbitals. Chemical Physics Letters, 2006, 418, 333-336.	2.6	13
86	CVRQD ab initio ground-state adiabatic potential energy surfaces for the water molecule. Journal of Chemical Physics, 2006, 125, 204307.	3.0	112
87	Chapter 2 Explicitly Correlated Approaches for Electronic Structure Computations. Annual Reports in Computational Chemistry, 2006, 2, 19-33.	1.7	4
88	Poster reception---Component architectures for quantum chemistry. , 2006, , .		0
89	Analysis of the errors in explicitly correlated electronic structure theory. Physical Chemistry Chemical Physics, 2005, 7, 2710.	2.8	120
90	HEAT: High accuracy extrapolatedab initiothermochemistry. Journal of Chemical Physics, 2004, 121, 11599-11613.	3.0	691

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91	Improving on the resolution of the identity in linear R12 ab initio theories. Chemical Physics Letters, 2004, 395, 190-195.	2.6	348
92	Second-order MÃ¸llerâ€“Plesset theory with linear R12 terms (MP2-R12) revisited: Auxiliary basis set method and massively parallel implementation. Journal of Chemical Physics, 2004, 121, 1214-1227.	3.0	67
93	A Comparison of One-Particle Basis Set Completeness, Higher-Order Electron Correlation, Relativistic Effects, and Adiabatic Corrections for Spectroscopic Constants of BH, CH+, and NHâ€. Journal of Physical Chemistry A, 2004, 108, 3068-3075.	2.5	32
94	The electron and nuclear orbitals model: current challenges and future prospects. Molecular Physics, 2004, 102, 111-123.	1.7	84
95	On the accuracy limits of orbital expansion methods: Explicit effects ofk-functions on atomic and molecular energies. Journal of Chemical Physics, 2003, 118, 8594-8610.	3.0	70
96	The diagonal Bornâ€“Oppenheimer correction beyond the Hartreeâ€“Fock approximation. Journal of Chemical Physics, 2003, 118, 3921-3927.	3.0	122
97	Three-â€‰versusâ€‰four-coordinateâ€‰phosphorusâ€‰inâ€‰theâ€‰gasâ€‰phaseâ€‰andâ€‰inâ€‰solution: Treacherous for phosphine oxide and phosphinousâ€‰acid. Journal of Chemical Physics, 2002, 116, 112.	3.0	27
98	Anchoring the water dimer potential energy surface with explicitly correlated computations and focal point analyses. Journal of Chemical Physics, 2002, 116, 690-701.	3.0	262
99	The Equilibrium Geometry, Harmonic Vibrational Frequencies, and Estimated ab Initio Limit for the Barrier to Planarity of the Ethylene Radical Cation. Journal of Physical Chemistry A, 2002, 106, 2671-2675.	2.5	18
100	Estimates of the Ab Initio Limit for Ï€â^Ï€ Interactions:â€‰ The Benzene Dimer. Journal of the American Chemical Society, 2002, 124, 10887-10893.	13.7	1,229
101	Interlocking Triplet Electronic States of Isocyanic Acid:Â Sources of Nonadiabatic Photofragmentation Dynamicsâ€. Journal of Physical Chemistry A, 2001, 105, 2716-2730.	2.5	14
102	The second-order MÃ¸llerâ€“Plesset limit for the barrier to linearity of water. Journal of Chemical Physics, 2001, 114, 2875-2878.	3.0	49
103	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
104	Evaluation of two-electron integrals for explicit r12 theories. Journal of Chemical Physics, 2000, 113, 3990-3995.	3.0	44
105	C60complexes with dianthracene and triptycene: synthesis and crystal structures. Synthetic Metals, 1999, 103, 2364-2365.	3.9	25
106	The protonated water dimer: Brueckner methods remove the spurious C1 symmetry minimum. Journal of Chemical Physics, 1998, 108, 7197-7201.	3.0	102
107	Is F3+ viable? A high-level ab initio comparison of F3+ and Cl3+. Journal of Chemical Physics, 1998, 109, 1772-1780.	3.0	6
108	A series of new molecular complexes C60(S4N4)2 â^' x(C6H6)x: Synthesis, x-ray study of crystal structure and structural disorder. Journal of Physics and Chemistry of Solids, 1997, 58, 1865-1867.	4.0	11

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109	The elementary reaction of quartet methylidyne (CH) with methane. Molecular Physics, 1996, 89, 1695-1705.	1.7	9
110	The elementary reaction of quartet methylidyne (CH) with methane. Molecular Physics, 1996, 89, 1695-1705.	1.7	0
111	EXAFS study of the M0.5(OH)x(H2O)yMoS2 intercalated complexes. Physica B: Condensed Matter, 1995, 208-209, 569-570.	2.7	6
112	An Introduction to High Performance Computing and Its Intersection with Advances in Modeling Rare Earth Elements and Actinides. ACS Symposium Series, 0, , 3-53.	0.5	3