

Edward F Valeev

List of Publications by Year in descending order

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111
papers

11,063
citations

71061

41
h-index

30058

103
g-index

113
all docs

113
docs citations

113
times ranked

8494
citing authors

#	ARTICLE	IF	CITATIONS
1	Estimates of the Ab Initio Limit for π - π Interactions: The Benzene Dimer. <i>Journal of the American Chemical Society</i> , 2002, 124, 10887-10893.	6.6	1,229
2	<sc>Psi4</sc> 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3185-3197.	2.3	961
3	Psi4: an open-source <i>ab initio</i> electronic structure program. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2012, 2, 556-565.	6.2	838
4	Effect of Electronic Polarization on Charge-Transport Parameters in Molecular Organic Semiconductors. <i>Journal of the American Chemical Society</i> , 2006, 128, 9882-9886.	6.6	756
5	Sparse maps: A systematic infrastructure for reduced-scaling electronic structure methods. II. Linear scaling domain based pair natural orbital coupled cluster theory. <i>Journal of Chemical Physics</i> , 2016, 144, 024109.	1.2	740
6	HEAT: High accuracy extrapolated <i>ab initio</i> thermochemistry. <i>Journal of Chemical Physics</i> , 2004, 121, 11599-11613.	1.2	691
7	Explicitly Correlated R12/F12 Methods for Electronic Structure. <i>Chemical Reviews</i> , 2012, 112, 75-107.	23.0	408
8	R12 methods in explicitly correlated molecular electronic structure theory. <i>International Reviews in Physical Chemistry</i> , 2006, 25, 427-468.	0.9	384
9	Improving on the resolution of the identity in linear R12 <i>ab initio</i> theories. <i>Chemical Physics Letters</i> , 2004, 395, 190-195.	1.2	348
10	A new near-linear scaling, efficient and accurate, open-shell domain-based local pair natural orbital coupled cluster singles and doubles theory. <i>Journal of Chemical Physics</i> , 2017, 146, 164105.	1.2	285
11	Revisiting the Atomic Natural Orbital Approach for Basis Sets: Robust Systematic Basis Sets for Explicitly Correlated and Conventional Correlated <i>ab initio</i> Methods?. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 33-43.	2.3	274
12	Anchoring the water dimer potential energy surface with explicitly correlated computations and focal point analyses. <i>Journal of Chemical Physics</i> , 2002, 116, 690-701.	1.2	262
13	PSI3: An open-source <i>Ab Initio</i> electronic structure package. <i>Journal of Computational Chemistry</i> , 2007, 28, 1610-1616.	1.5	258
14	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. <i>Journal of Chemical Physics</i> , 2015, 143, 034108.	1.2	211
15	SparseMaps: A systematic infrastructure for reduced-scaling electronic structure methods. III. Linear-scaling multireference domain-based pair natural orbital N-electron valence perturbation theory. <i>Journal of Chemical Physics</i> , 2016, 144, 094111.	1.2	131
16	The diagonal Born-Oppenheimer correction beyond the Hartree-Fock approximation. <i>Journal of Chemical Physics</i> , 2003, 118, 3921-3927.	1.2	122
17	SparseMaps: A systematic infrastructure for reduced scaling electronic structure methods. V. Linear scaling explicitly correlated coupled-cluster method with pair natural orbitals. <i>Journal of Chemical Physics</i> , 2017, 146, 174108.	1.2	122
18	Analysis of the errors in explicitly correlated electronic structure theory. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 2710.	1.3	120

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19	Simple coupled-cluster singles and doubles method with perturbative inclusion of triples and explicitly correlated geminals: The CCSD(T)R12 \tilde{A} model. <i>Journal of Chemical Physics</i> , 2008, 128, 244113.	1.2	113
20	CVRQD ab initio ground-state adiabatic potential energy surfaces for the water molecule. <i>Journal of Chemical Physics</i> , 2006, 125, 204307.	1.2	112
21	Coupled-cluster methods with perturbative inclusion of explicitly correlated terms: a preliminary investigation. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 106-113.	1.3	106
22	The protonated water dimer: Brueckner methods remove the spurious C1 symmetry minimum. <i>Journal of Chemical Physics</i> , 1998, 108, 7197-7201.	1.2	102
23	SparseMaps – A systematic infrastructure for reduced-scaling electronic structure methods. IV. Linear-scaling second-order explicitly correlated energy with pair natural orbitals. <i>Journal of Chemical Physics</i> , 2016, 144, 144109.	1.2	98
24	Explicitly correlated coupled-cluster singles and doubles method based on complete diagrammatic equations. <i>Journal of Chemical Physics</i> , 2008, 129, 071101.	1.2	94
25	Adaptive Steered Molecular Dynamics of the Long-Distance Unfolding of Neuropeptide Y. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3026-3038.	2.3	88
26	Variational formulation of perturbative explicitly-correlated coupled-cluster methods. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 3410.	1.3	85
27	The electron and nuclear orbitals model: current challenges and future prospects. <i>Molecular Physics</i> , 2004, 102, 111-123.	0.8	84
28	Prediction of Reaction Barriers and Thermochemical Properties with Explicitly Correlated Coupled-Cluster Methods: A Basis Set Assessment. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3175-3186.	2.3	79
29	Equations of explicitly-correlated coupled-cluster methods. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 3358.	1.3	77
30	Higher-order explicitly correlated coupled-cluster methods. <i>Journal of Chemical Physics</i> , 2009, 130, 054101.	1.2	73
31	MADNESS: A Multiresolution, Adaptive Numerical Environment for Scientific Simulation. <i>SIAM Journal of Scientific Computing</i> , 2016, 38, S123-S142.	1.3	72
32	On the accuracy limits of orbital expansion methods: Explicit effects of k -functions on atomic and molecular energies. <i>Journal of Chemical Physics</i> , 2003, 118, 8594-8610.	1.2	70
33	Universal perturbative explicitly correlated basis set incompleteness correction. <i>Journal of Chemical Physics</i> , 2009, 131, 171103.	1.2	70
34	Second-order \tilde{M} -Plesset theory with linear R12 terms (MP2-R12) revisited: Auxiliary basis set method and massively parallel implementation. <i>Journal of Chemical Physics</i> , 2004, 121, 1214-1227.	1.2	67
35	The Chronus Quantum software package. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2020, 10, e1436.	6.2	66
36	Combining explicitly correlated R12 and Gaussian geminal electronic structure theories. <i>Journal of Chemical Physics</i> , 2006, 125, 244106.	1.2	59

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37	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 H ₂ O, N ₂ H ⁺ , NO ₂ ⁺ , and C ₂ H ₂ . <i>Journal of Chemical Physics</i> , 2010, 133, 244108.	1.2	55
38	Massively Parallel Implementation of Explicitly Correlated Coupled-Cluster Singles and Doubles Using TiledArray Framework. <i>Journal of Physical Chemistry A</i> , 2016, 120, 10231-10244.	1.1	50
39	The second-order Møller-Plesset limit for the barrier to linearity of water. <i>Journal of Chemical Physics</i> , 2001, 114, 2875-2878.	1.2	49
40	Evaluation of two-electron integrals for explicit r ₁₂ theories. <i>Journal of Chemical Physics</i> , 2000, 113, 3990-3995.	1.2	44
41	Quantum simulation of electronic structure with a transcorrelated Hamiltonian: improved accuracy with a smaller footprint on the quantum computer. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 24270-24281.	1.3	43
42	Low-order tensor approximations for electronic wave functions: Hartree-Fock method with guaranteed precision. <i>Journal of Chemical Physics</i> , 2011, 134, 104104.	1.2	42
43	Computing many-body wave functions with guaranteed precision: The first-order Møller-Plesset wave function for the ground state of helium atom. <i>Journal of Chemical Physics</i> , 2012, 137, 104103.	1.2	40
44	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. <i>Chemical Reviews</i> , 2021, 121, 4962-4998.	23.0	39
45	Efficient implementation of the analytic second derivatives of Hartree-Fock and hybrid DFT energies: a detailed analysis of different approximations. <i>Molecular Physics</i> , 2015, 113, 1961-1977.	0.8	38
46	Coupled-cluster singles, doubles and perturbative triples with density fitting approximation for massively parallel heterogeneous platforms. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25894.	1.0	37
47	Geminal-spanning orbitals make explicitly correlated reduced-scaling coupled-cluster methods robust, yet simple. <i>Journal of Chemical Physics</i> , 2014, 141, 054106.	1.2	36
48	Explicitly correlated combined coupled-cluster and perturbation methods. <i>Journal of Chemical Physics</i> , 2009, 131, 044118.	1.2	33
49	What is the most efficient way to reach the canonical MP2 basis set limit?. <i>Molecular Physics</i> , 2013, 111, 2653-2662.	0.8	33
50	Semi-exact concentric atomic density fitting: Reduced cost and increased accuracy compared to standard density fitting. <i>Journal of Chemical Physics</i> , 2014, 140, 064109.	1.2	33
51	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. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3068-3075.	1.1	32
52	State-Averaged Pair Natural Orbitals for Excited States: A Route toward Efficient Equation of Motion Coupled-Cluster. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5597-5607.	2.3	32
53	Computing molecular correlation energies with guaranteed precision. <i>Journal of Chemical Physics</i> , 2013, 139, 114106.	1.2	31
54	Perturbative correction for the basis set incompleteness error of complete-active-space self-consistent field. <i>Journal of Chemical Physics</i> , 2010, 133, 174126.	1.2	30

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55	$\$ \text{box}\{\text{SF-}[2]\}_{\text{ext}\{\text{R12}\}} \text{ SF-}[2] \text{ R12}$: A spin-adapted explicitly correlated method applicable to arbitrary electronic states. <i>Journal of Chemical Physics</i> , 2011, 135, 214105.	1.2	29
56	Three- versus four-coordinate phosphorus in the gas phase and in solution: Treacherous re for phosphine oxide and phosphinous acid. <i>Journal of Chemical Physics</i> , 2002, 116, 112.	1.2	27
57	(1,2-Diaminoethane-1,2-diyl)bis(N-methylpyridinium) Salts as a Prospective Platform for Designing Recyclable Prolinamide-Based Organocatalysts. <i>Journal of Organic Chemistry</i> , 2015, 80, 9570-9577.	1.7	26
58	C60 complexes with dianthracene and triptycene: synthesis and crystal structures. <i>Synthetic Metals</i> , 1999, 103, 2364-2365.	2.1	25
59	Massively Parallel Quantum Chemistry: A high-performance research platform for electronic structure. <i>Journal of Chemical Physics</i> , 2020, 153, 044120.	1.2	25
60	Chapter 6 Explicitly Correlated Coupled-Cluster Methods. <i>Annual Reports in Computational Chemistry</i> , 2009, , 131-148.	0.9	24
61	A novel interpretation of reduced density matrix and cumulant for electronic structure theories. <i>Journal of Chemical Physics</i> , 2011, 134, 214109.	1.2	24
62	Efficient Four-Component Dirac-Coulomb-Gaunt Hartree-Fock in the Pauli Spinor Representation. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3388-3402.	2.3	24
63	Explicitly correlated coupled cluster method for accurate treatment of open-shell molecules with hundreds of atoms. <i>Journal of Chemical Physics</i> , 2020, 153, 094105.	1.2	22
64	Components for integral evaluation in quantum chemistry. <i>Journal of Computational Chemistry</i> , 2008, 29, 562-577.	1.5	21
65	Many-Body Quantum Chemistry on Massively Parallel Computers. <i>Chemical Reviews</i> , 2021, 121, 1203-1231.	23.0	21
66	Is the adiabatic approximation sufficient to account for the post-Born-Oppenheimer effects on molecular electric dipole moments?. <i>Molecular Physics</i> , 2009, 107, 1153-1159.	0.8	20
67	Scalar relativistic explicitly correlated R12 methods. <i>Journal of Chemical Physics</i> , 2010, 132, 214104.	1.2	20
68	Clustered Low-Rank Tensor Format: Introduction and Application to Fast Construction of Hartree-Fock Exchange. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5868-5880.	2.3	20
69	Explicitly correlated N-electron valence state perturbation theory (NEVPT2-F12). <i>Journal of Chemical Physics</i> , 2017, 147, 064110.	1.2	20
70	The Equilibrium Geometry, Harmonic Vibrational Frequencies, and Estimated ab Initio Limit for the Barrier to Planarity of the Ethylene Radical Cation. <i>Journal of Physical Chemistry A</i> , 2002, 106, 2671-2675.	1.1	18
71	Communication: Stochastic evaluation of explicitly correlated second-order many-body perturbation energy. <i>Journal of Chemical Physics</i> , 2014, 140, 031101.	1.2	18
72	Scalable task-based algorithm for multiplication of block-rank-sparse matrices. , 2015, , .		18

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73	A tight distance-dependent estimator for screening three-center Coulomb integrals over Gaussian basis functions. <i>Journal of Chemical Physics</i> , 2015, 142, 154106.	1.2	18
74	Developing a Computational Chemistry Framework for the Exascale Era. <i>Computing in Science and Engineering</i> , 2019, 21, 48-58.	1.2	16
75	Explicitly correlated second-order Møller-Plesset perturbation theory in a Divide-Expand-Consolidate (DEC) context. <i>Journal of Chemical Physics</i> , 2016, 144, 204112.	1.2	15
76	Direct determination of optimal pair-natural orbitals in a real-space representation: The second-order Møller-Plesset energy. <i>Journal of Chemical Physics</i> , 2020, 152, 074105.	1.2	15
77	Interlocking Triplet Electronic States of Isocyanic Acid: Sources of Nonadiabatic Photofragmentation Dynamics. <i>Journal of Physical Chemistry A</i> , 2001, 105, 2716-2730.	1.1	14
78	Computation of precise two-electron correlation energies with imprecise Hartree-Fock orbitals. <i>Chemical Physics Letters</i> , 2006, 418, 333-336.	1.2	13
79	Monte Carlo explicitly correlated second-order many-body perturbation theory. <i>Journal of Chemical Physics</i> , 2016, 145, 154115.	1.2	13
80	Communication: Explicitly correlated formalism for second-order single-particle Green's function. <i>Journal of Chemical Physics</i> , 2017, 147, 121101.	1.2	13
81	Optimized Pair Natural Orbitals for the Coupled Cluster Methods. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4581-4589.	2.3	13
82	Can the distinguishable cluster approximation be improved systematically by including connected triples?. <i>Journal of Chemical Physics</i> , 2019, 151, .	1.2	13
83	Enabling new capabilities and insights from quantum chemistry by using component architectures. <i>Journal of Physics: Conference Series</i> , 2006, 46, 220-228.	0.3	12
84	A New Class of Supramolecular Wires. <i>Journal of Physical Chemistry C</i> , 2007, 111, 18912-18916.	1.5	12
85	Efficient evaluation of exact exchange for periodic systems via concentric atomic density fitting. <i>Journal of Chemical Physics</i> , 2020, 153, 124116.	1.2	12
86	A series of new molecular complexes $C_{60}(S_4N_4)_2 \cdot x(C_6H_6)_x$: Synthesis, x-ray study of crystal structure and structural disorder. <i>Journal of Physics and Chemistry of Solids</i> , 1997, 58, 1865-1867.	1.9	11
87	Toward the Minimal Floating Operation Count Cholesky Decomposition of Electron Repulsion Integrals. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4258-4265.	1.1	11
88	The not-so-peculiar case of calcium oxide: a weakness in atomic natural orbital basis sets for calcium. <i>Molecular Physics</i> , 2000, 98, 1227-1231.	0.8	10
89	Assessment of Perturbative Explicitly Correlated Methods for Prototypes of Multiconfiguration Electronic Structure. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 90-101.	2.3	10
90	The elementary reaction of quartet methylidyne (CH) with methane. <i>Molecular Physics</i> , 1996, 89, 1695-1705.	0.8	9

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91	Robust Approximation of Tensor Networks: Application to Grid-Free Tensor Factorization of the Coulomb Interaction. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2217-2230.	2.3	8
92	Effective Utilization of Tensor Symmetry in Operation Optimization of Tensor Contraction Expressions. <i>Procedia Computer Science</i> , 2012, 9, 412-421.	1.2	7
93	EXAFS study of the $M_{0.5}(OH)_x(H_2O)_yMoS_2$ intercalated complexes. <i>Physica B: Condensed Matter</i> , 1995, 208-209, 569-570.	1.3	6
94	Is $F3+$ viable? A high-level ab initio comparison of $F3+$ and $Cl3+$. <i>Journal of Chemical Physics</i> , 1998, 109, 1772-1780.	1.2	6
95	Anatomy of molecular properties evaluated with explicitly correlated electronic wave functions. <i>Molecular Physics</i> , 2016, 114, 2894-2909.	0.8	6
96	Explicitly correlated renormalized second-order Green's function for accurate ionization potentials of closed-shell molecules. <i>Journal of Chemical Physics</i> , 2019, 150, 214103.	1.2	6
97	The Template Task Graph (TTG) - an emerging practical dataflow programming paradigm for scientific simulation at extreme scale. , 2020, , .		6
98	Fast construction of the exchange operator in an atom-centred basis with concentric atomic density fitting. <i>Molecular Physics</i> , 2017, 115, 2065-2076.	0.8	5
99	Combined Relativistic Ab Initio Multireference and Experimental Study of the Electronic Structure of Terbium Luminescent Compound. <i>Journal of Physical Chemistry A</i> , 2020, 124, 82-89.	1.1	5
100	Chapter 2 Explicitly Correlated Approaches for Electronic Structure Computations. <i>Annual Reports in Computational Chemistry</i> , 2006, 2, 19-33.	0.9	4
101	Distributed-memory multi-GPU block-sparse tensor contraction for electronic structure. , 2021, , .		4
102	Hybrid one-electron/many-electron methods for ionized states of molecular clusters. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 7863.	1.3	3
103	Spin-Free [2] R_{12} Basis Set Incompleteness Correction to the Local Multireference Configuration Interaction and the Local Multireference Average Coupled Pair Functional Methods. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3176-3184.	2.3	3
104	An Introduction to High Performance Computing and Its Intersection with Advances in Modeling Rare Earth Elements and Actinides. <i>ACS Symposium Series</i> , 0, , 3-53.	0.5	3
105	Comment on "A tight distance-dependent estimator for screening three-center Coulomb integrals over Gaussian basis functions" [J. Chem. Phys. 142, 154106 (2015)]. <i>Journal of Chemical Physics</i> , 2020, 153, 097101.	1.2	2
106	Robust Pipek-Mezey Orbital Localization in Periodic Solids. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7406-7415.	2.3	2
107	Generalized Flow-Graph Programming Using Template Task-Graphs: Initial Implementation and Assessment. , 2022, , .		2
108	Molecular Resonance Raman and Rayleigh Scattering Stimulated by a Short Laser Pulse. <i>Journal of Statistical Physics</i> , 2014, 154, 522-542.	0.5	1

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109	Poster reception--Component architectures for quantum chemistry. , 2006, , .		0
110	Computational Interstellar Chemistry. Thirty Years of Astronomical Discovery With UKIRT, 2010, , 21-30.	0.3	0
111	Eclectic Electron-Correlation Methods. Challenges and Advances in Computational Chemistry and Physics, 2010, , 191-217.	0.6	0