

Edward F Valeev

List of Publications by Year in Descending Order

Source: <https://exaly.com/author-pdf/2357877/edward-f-valeev-publications-by-year.pdf>

Version: 2024-04-28

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. <i>Chemical Reviews</i> , 2021 , 121, 4962-4998	68.1	12
105	Toward the Minimal Floating Operation Count Cholesky Decomposition of Electron Repulsion Integrals. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 4258-4265	2.8	0
104	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	6.4	4
103	Many-Body Quantum Chemistry on Massively Parallel Computers. <i>Chemical Reviews</i> , 2021 , 121, 1203-1238	68.1	6
102	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	6.4	4
101	Direct determination of optimal pair-natural orbitals in a real-space representation: The second-order Moller-Plesset energy. <i>Journal of Chemical Physics</i> , 2020 , 152, 074105	3.9	5
100	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	2.8	2
99	Massively Parallel Quantum Chemistry: A high-performance research platform for electronic structure. <i>Journal of Chemical Physics</i> , 2020 , 153, 044120	3.9	12
98	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	3.6	11
97	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	3.9	4
96	Efficient evaluation of exact exchange for periodic systems via concentric atomic density fitting. <i>Journal of Chemical Physics</i> , 2020 , 153, 124116	3.9	3
95	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	3.9	1
94	The Chronus Quantum software package. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2020 , 10, e1436	7.9	31
93	Can the distinguishable cluster approximation be improved systematically by including connected triples?. <i>Journal of Chemical Physics</i> , 2019 , 151, 064102	3.9	7
92	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	3.9	6
91	. <i>Computing in Science and Engineering</i> , 2019 , 21, 48-58	1.5	7
90	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	2.1	28

89	Optimized Pair Natural Orbitals for the Coupled Cluster Methods. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 4581-4589	6.4	11
88	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	6.4	24
87	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	3.9	84
86	Psi4 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	6.4	733
85	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	3.9	194
84	Communication: Explicitly correlated formalism for second-order single-particle Green's function. <i>Journal of Chemical Physics</i> , 2017 , 147, 121101	3.9	12
83	Fast construction of the exchange operator in an atom-centred basis with concentric atomic density fitting. <i>Molecular Physics</i> , 2017 , 115, 2065-2076	1.7	5
82	Explicitly correlated N-electron valence state perturbation theory (NEVPT2-F12). <i>Journal of Chemical Physics</i> , 2017 , 147, 064110	3.9	13
81	MADNESS: A Multiresolution, Adaptive Numerical Environment for Scientific Simulation. <i>SIAM Journal of Scientific Computing</i> , 2016 , 38, S123-S142	2.6	48
80	Spin-Free [2]R12 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, 3176-84	6.4	2
79	Anatomy of molecular properties evaluated with explicitly correlated electronic wave functions. <i>Molecular Physics</i> , 2016 , 114, 2894-2909	1.7	5
78	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	6.4	17
77	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	3.9	105
76	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	3.9	77
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	3.9	10
74	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	2.8	39
73	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	3.9	489
72	Monte Carlo explicitly correlated second-order many-body perturbation theory. <i>Journal of Chemical Physics</i> , 2016 , 145, 154115	3.9	12

71	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	1.7	27
70	A tight distance-dependent estimator for screening three-center Coulomb integrals over Gaussian basis functions. <i>Journal of Chemical Physics</i> , 2015 , 142, 154106	3.9	16
69	(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, 9570-7	4.2	22
68	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	3.9	169
67	Scalable task-based algorithm for multiplication of block-rank-sparse matrices 2015 ,		9
66	Molecular Resonance Raman and Rayleigh Scattering Stimulated by a Short Laser Pulse. <i>Journal of Statistical Physics</i> , 2014 , 154, 522-542	1.5	1
65	Assessment of Perturbative Explicitly Correlated Methods for Prototypes of Multiconfiguration Electronic Structure. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 90-101	6.4	8
64	Geminal-spanning orbitals make explicitly correlated reduced-scaling coupled-cluster methods robust, yet simple. <i>Journal of Chemical Physics</i> , 2014 , 141, 054106	3.9	33
63	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	3.9	29
62	Communication: stochastic evaluation of explicitly correlated second-order many-body perturbation energy. <i>Journal of Chemical Physics</i> , 2014 , 140, 031101	3.9	17
61	Computing molecular correlation energies with guaranteed precision. <i>Journal of Chemical Physics</i> , 2013 , 139, 114106	3.9	29
60	What is the most efficient way to reach the canonical MP2 basis set limit?. <i>Molecular Physics</i> , 2013 , 111, 2653-2662	1.7	30
59	Explicitly correlated R12/F12 methods for electronic structure. <i>Chemical Reviews</i> , 2012 , 112, 75-107	68.1	334
58	Effective Utilization of Tensor Symmetry in Operation Optimization of Tensor Contraction Expressions. <i>Procedia Computer Science</i> , 2012 , 9, 412-421	1.6	4
57	Hybrid one-electron/many-electron methods for ionized states of molecular clusters. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 7863-71	3.6	3
56	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, 3175-86	6.4	56
55	Computing many-body wave functions with guaranteed precision: the first-order Müller-Plesset wave function for the ground state of helium atom. <i>Journal of Chemical Physics</i> , 2012 , 137, 104103	3.9	34
54	Psi4: an open-source ab initio electronic structure program. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2012 , 2, 556-565	7.9	678

53	A novel interpretation of reduced density matrix and cumulant for electronic structure theories. <i>Journal of Chemical Physics</i> , 2011 , 134, 214109	3.9	22
52	Revisiting the Atomic Natural Orbital Approach for Basis Sets: Robust Systematic Basis Sets for Explicitly Correlated and Conventional Correlated ab initio Methods?. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 33-43	6.4	195
51	Low-order tensor approximations for electronic wave functions: Hartree-Fock method with guaranteed precision. <i>Journal of Chemical Physics</i> , 2011 , 134, 104104	3.9	35
50	SF-[2]R12: a spin-adapted explicitly correlated method applicable to arbitrary electronic states. <i>Journal of Chemical Physics</i> , 2011 , 135, 214105	3.9	26
49	Scalar relativistic explicitly correlated R12 methods. <i>Journal of Chemical Physics</i> , 2010 , 132, 214104	3.9	17
48	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	3.9	42
47	Adaptive Steered Molecular Dynamics of the Long-Distance Unfolding of Neuropeptide Y. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 3026-38	6.4	58
46	Perturbative correction for the basis set incompleteness error of complete-active-space self-consistent field. <i>Journal of Chemical Physics</i> , 2010 , 133, 174126	3.9	29
45	Computational Interstellar Chemistry. <i>Thirty Years of Astronomical Discovery With UKIRT</i> , 2010 , 21-30	0.3	
44	Eclectic Electron-Correlation Methods. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2010 , 191-217	0.7	
43	Higher-order explicitly correlated coupled-cluster methods. <i>Journal of Chemical Physics</i> , 2009 , 130, 054101	3.9	71
42	Chapter 6 Explicitly Correlated Coupled-Cluster Methods. <i>Annual Reports in Computational Chemistry</i> , 2009 , 131-148	1.8	24
41	Explicitly correlated combined coupled-cluster and perturbation methods. <i>Journal of Chemical Physics</i> , 2009 , 131, 044118	3.9	33
40	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	1.7	18
39	Universal perturbative explicitly correlated basis set incompleteness correction. <i>Journal of Chemical Physics</i> , 2009 , 131, 171103	3.9	63
38	Equations of explicitly-correlated coupled-cluster methods. <i>Physical Chemistry Chemical Physics</i> , 2008 , 10, 3358-70	3.6	70
37	Explicitly correlated coupled-cluster singles and doubles method based on complete diagrammatic equations. <i>Journal of Chemical Physics</i> , 2008 , 129, 071101	3.9	87
36	Simple coupled-cluster singles and doubles method with perturbative inclusion of triples and explicitly correlated geminals: The CCSD(T)R12 model. <i>Journal of Chemical Physics</i> , 2008 , 128, 244113	3.9	99

35	Variational formulation of perturbative explicitly-correlated coupled-cluster methods. <i>Physical Chemistry Chemical Physics</i> , 2008 , 10, 3410-20	3.6	77
34	Coupled-cluster methods with perturbative inclusion of explicitly correlated terms: a preliminary investigation. <i>Physical Chemistry Chemical Physics</i> , 2008 , 10, 106-13	3.6	94
33	Components for integral evaluation in quantum chemistry. <i>Journal of Computational Chemistry</i> , 2008 , 29, 562-77	3.5	14
32	PSI3: an open-source Ab Initio electronic structure package. <i>Journal of Computational Chemistry</i> , 2007 , 28, 1610-1616	3.5	249
31	A New Class of Supramolecular Wires. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 18912-18916	3.8	11
30	CVRQD ab initio ground-state adiabatic potential energy surfaces for the water molecule. <i>Journal of Chemical Physics</i> , 2006 , 125, 204307	3.9	106
29	Chapter 2 Explicitly Correlated Approaches for Electronic Structure Computations. <i>Annual Reports in Computational Chemistry</i> , 2006 , 2, 19-33	1.8	4
28	Combining explicitly correlated R12 and Gaussian geminal electronic structure theories. <i>Journal of Chemical Physics</i> , 2006 , 125, 244106	3.9	59
27	Effect of electronic polarization on charge-transport parameters in molecular organic semiconductors. <i>Journal of the American Chemical Society</i> , 2006 , 128, 9882-6	16.4	652
26	R12 methods in explicitly correlated molecular electronic structure theory. <i>International Reviews in Physical Chemistry</i> , 2006 , 25, 427-468	7	360
25	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
24	Computation of precise two-electron correlation energies with imprecise Hartree-Fock orbitals. <i>Chemical Physics Letters</i> , 2006 , 418, 333-336	2.5	13
23	Analysis of the errors in explicitly correlated electronic structure theory. <i>Physical Chemistry Chemical Physics</i> , 2005 , 7, 2710-3	3.6	113
22	HEAT: High accuracy extrapolated ab initio thermochemistry. <i>Journal of Chemical Physics</i> , 2004 , 121, 11599-613	3.9	606
21	Improving on the resolution of the identity in linear R12 ab initio theories. <i>Chemical Physics Letters</i> , 2004 , 395, 190-195	2.5	318
20	Second-order Møller-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, 1214-27	3.9	64
19	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 ₂ ⁺ . <i>Journal of Physical Chemistry A</i> , 2004 , 108, 3068-3075	2.8	28
18	The electron and nuclear orbitals model: current challenges and future prospects. <i>Molecular Physics</i> , 2004 , 102, 111-123	1.7	72

17	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	3.9	68
16	The diagonal Born-Oppenheimer correction beyond the Hartree-Fock approximation. <i>Journal of Chemical Physics</i> , 2003 , 118, 3921-3927	3.9	113
15	Estimates of the ab initio limit for pi-pi interactions: the benzene dimer. <i>Journal of the American Chemical Society</i> , 2002 , 124, 10887-93	16.4	1112
14	Three- versus four-coordinate phosphorus in the gas phase and in solution: Treacherous relative energies for phosphine oxide and phosphinous acid. <i>Journal of Chemical Physics</i> , 2002 , 116, 112	3.9	25
13	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	3.9	239
12	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	2.8	17
11	The second-order Møller-Plesset limit for the barrier to linearity of water. <i>Journal of Chemical Physics</i> , 2001 , 114, 2875-2878	3.9	47
10	Interlocking Triplet Electronic States of Isocyanic Acid: Sources of Nonadiabatic Photofragmentation Dynamics. <i>Journal of Physical Chemistry A</i> , 2001 , 105, 2716-2730	2.8	14
9	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	1.7	10
8	Evaluation of two-electron integrals for explicit r12 theories. <i>Journal of Chemical Physics</i> , 2000 , 113, 3990-3995	3.9	43
7	C60 complexes with dianthracene and triptycene: synthesis and crystal structures. <i>Synthetic Metals</i> , 1999 , 103, 2364-2365	3.6	22
6	The protonated water dimer: Brueckner methods remove the spurious C1 symmetry minimum. <i>Journal of Chemical Physics</i> , 1998 , 108, 7197-7201	3.9	98
5	Is F3+ viable? A high-level ab initio comparison of F3+ and Cl3+. <i>Journal of Chemical Physics</i> , 1998 , 109, 1772-1780	3.9	6
4	A series of new molecular complexes C60(S4N4)2 · x(C6H6)x: Synthesis, x-ray study of crystal structure and structural disorder. <i>Journal of Physics and Chemistry of Solids</i> , 1997 , 58, 1865-1867	3.9	10
3	The elementary reaction of quartet methylidyne (CH) with methane. <i>Molecular Physics</i> , 1996 , 89, 1695-1705	3.9	8
2	EXAFS study of the M0.5(OH)x(H2O)yMoS2 intercalated complexes. <i>Physica B: Condensed Matter</i> , 1995 , 208-209, 569-570	2.8	6
1	An Introduction to High Performance Computing and Its Intersection with Advances in Modeling Rare Earth Elements and Actinides. <i>ACS Symposium Series</i> , 3-53	0.4	0