# 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 | 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 |
| 2 | <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 |
| 3 | Psi4: an openâ€source ab initio electronic structure program. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 556-565. | 14.6 | 838 |
| 4 | 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 |
| 5 | 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 |
| 6 | HEAT: High accuracy extrapolatedab initiothermochemistry. Journal of Chemical Physics, 2004, 121, 11599-11613. | 3.0 | 691 |
| 7 | Explicitly Correlated R12/F12 Methods for Electronic Structure. Chemical Reviews, 2012, 112, 75-107. | 47.7 | 408 |
| 8 | R12 methods in explicitly correlated molecular electronic structure theory. International Reviews in Physical Chemistry, 2006, 25, 427-468. | 2.3 | 384 |
| 9 | Improving on the resolution of the identity in linear R12 ab initio theories. Chemical Physics Letters, 2004, 395, 190-195. | 2.6 | 348 |
| 10 | 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 |
| 11 | 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 |
| 12 | 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 |
| 13 | PSI3: An open-source Ab Initio electronic structure package. Journal of Computational Chemistry, 2007, 28, 1610-1616. | 3.3 | 258 |
| 14 | 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 |
| 15 | 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 |
| 16 | The diagonal Bornâ€“Oppenheimer correction beyond the Hartreeâ€“Fock approximation. Journal of Chemical Physics, 2003, 118, 3921-3927. | 3.0 | 122 |
| 17 | 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 |
| 18 | Analysis of the errors in explicitly correlated electronic structure theory. Physical Chemistry Chemical Physics, 2005, 7, 2710. | 2.8 | 120 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | 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 |
| 20 | CVRQD ab initio ground-state adiabatic potential energy surfaces for the water molecule. Journal of Chemical Physics, 2006, 125, 204307. | 3.0 | 112 |
| 21 | Coupled-cluster methods with perturbative inclusion of explicitly correlated terms: a preliminary investigation. Physical Chemistry Chemical Physics, 2008, 10, 106-113. | 2.8 | 106 |
| 22 | The protonated water dimer: Brueckner methods remove the spurious C1 symmetry minimum. Journal of Chemical Physics, 1998, 108, 7197-7201. | 3.0 | 102 |
| 23 | 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 |
| 24 | Explicitly correlated coupled-cluster singles and doubles method based on complete diagrammatic equations. Journal of Chemical Physics, 2008, 129, 071101. | 3.0 | 94 |
| 25 | 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 |
| 26 | Variational formulation of perturbative explicitly-correlated coupled-cluster methods. Physical Chemistry Chemical Physics, 2008, 10, 3410. | 2.8 | 85 |
| 27 | The electron and nuclear orbitals model: current challenges and future prospects. Molecular Physics, 2004, 102, 111-123. | 1.7 | 84 |
| 28 | 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 |
| 29 | Equations of explicitly-correlated coupled-cluster methods. Physical Chemistry Chemical Physics, 2008, 10, 3358. | 2.8 | 77 |
| 30 | Higher-order explicitly correlated coupled-cluster methods. Journal of Chemical Physics, 2009, 130, 054101. | 3.0 | 73 |
| 31 | MADNESS: A Multiresolution, Adaptive Numerical Environment for Scientific Simulation. SIAM Journal of Scientific Computing, 2016, 38, S123-S142. | 2.8 | 72 |
| 32 | 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 |
| 33 | Universal perturbative explicitly correlated basis set incompleteness correction. Journal of Chemical Physics, 2009, 131, 171103. | 3.0 | 70 |
| 34 | 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 |
| 35 | The Chronus Quantum software package. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1436. | 14.6 | 66 |
| 36 | Combining explicitly correlated R12 and Gaussian geminal electronic structure theories. Journal of Chemical Physics, 2006, 125, 244106. | 3.0 | 59 |

| # | Article | IF | Citations |
|---|---|---|---|
| 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 H2O, N2H+, NO2+, and C2H2. Journal of Chemical Physics, 2010, 133, 244108. | 3.0 | 55 |
| 38 | 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 |
| 39 | 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 |
| 40 | Evaluation of two-electron integrals for explicit r12 theories. Journal of Chemical Physics, 2000, 113, 3990-3995. | 3.0 | 44 |
| 41 | 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 |
| 42 | Low-order tensor approximations for electronic wave functions: Hartreeâ€“Fock method with guaranteed precision. Journal of Chemical Physics, 2011, 134, 104104. | 3.0 | 42 |
| 43 | 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 |
| 44 | From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998. | 47.7 | 39 |
| 45 | 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 |
| 46 | 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 |
| 47 | Geminal-spanning orbitals make explicitly correlated reduced-scaling coupled-cluster methods robust, yet simple. Journal of Chemical Physics, 2014, 141, 054106. | 3.0 | 36 |
| 48 | Explicitly correlated combined coupled-cluster and perturbation methods. Journal of Chemical Physics, 2009, 131, 044118. | 3.0 | 33 |
| 49 | What is the most efficient way to reach the canonical MP2 basis set limit?. Molecular Physics, 2013, 111, 2653-2662. | 1.7 | 33 |
| 50 | 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 |
| 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 NHâ€. Journal of Physical Chemistry A, 2004, 108, 3068-3075. | 2.5 | 32 |
| 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. | 5.3 | 32 |
| 53 | Computing molecular correlation energies with guaranteed precision. Journal of Chemical Physics, 2013, 139, 114106. | 3.0 | 31 |
| 54 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | $hbox{SF-[2]}_{ext{R12}}$ SF-[2] R12 : A spin-adapted explicitly correlated method applicable to arbitrary electronic states. Journal of Chemical Physics, 2011, 135, 214105. | 3.0 | 29 |
| 56 | Three-â€‰versusâ€‰four-coordinateâ€‰phosphorusâ€‰inâ€‰theâ€‰gasâ€‰phaseâ€‰andâ€‰inâ€‰solution: Treacherous re for phosphine oxide and phosphinousâ€‰acid. Journal of Chemical Physics, 2002, 116, 112. | 3.0 | 27 |
| 57 | (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 |
| 58 | C60complexes with dianthracene and triptycene: synthesis and crystal structures. Synthetic Metals, 1999, 103, 2364-2365. | 3.9 | 25 |
| 59 | Massively Parallel Quantum Chemistry: A high-performance research platform for electronic structure. Journal of Chemical Physics, 2020, 153, 044120. | 3.0 | 25 |
| 60 | Chapter 6 Explicitly Correlated Coupled-Cluster Methods. Annual Reports in Computational Chemistry, 2009, , 131-148. | 1.7 | 24 |
| 61 | A novel interpretation of reduced density matrix and cumulant for electronic structure theories. Journal of Chemical Physics, 2011, 134, 214109. | 3.0 | 24 |
| 62 | 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 |
| 63 | 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 |
| 64 | Components for integral evaluation in quantum chemistry. Journal of Computational Chemistry, 2008, 29, 562-577. | 3.3 | 21 |
| 65 | Many-Body Quantum Chemistry on Massively Parallel Computers. Chemical Reviews, 2021, 121, 1203-1231. | 47.7 | 21 |
| 66 | 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 |
| 67 | Scalar relativistic explicitly correlated R12 methods. Journal of Chemical Physics, 2010, 132, 214104. | 3.0 | 20 |
| 68 | 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 |
| 69 | Explicitly correlated N-electron valence state perturbation theory (NEVPT2-F12). Journal of Chemical Physics, 2017, 147, 064110. | 3.0 | 20 |
| 70 | 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 |
| 71 | Communication: Stochastic evaluation of explicitly correlated second-order many-body perturbation energy. Journal of Chemical Physics, 2014, 140, 031101. | 3.0 | 18 |
| 72 | Scalable task-based algorithm for multiplication of block-rank-sparse matrices. , 2015, , . | | 18 |

| # | Article | IF | Citations |
|---|---|---|---|
| 73 | 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 |
| 74 | Developing a Computational Chemistry Framework for the Exascale Era. Computing in Science and Engineering, 2019, 21, 48-58. | 1.2 | 16 |
| 75 | 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 |
| 76 | 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 |
| 77 | 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 |
| 78 | Computation of precise two-electron correlation energies with imprecise Hartreeâ€“Fock orbitals. Chemical Physics Letters, 2006, 418, 333-336. | 2.6 | 13 |
| 79 | Monte Carlo explicitly correlated second-order many-body perturbation theory. Journal of Chemical Physics, 2016, 145, 154115. | 3.0 | 13 |
| 80 | Communication: Explicitly correlated formalism for second-order single-particle Greenâ€™s function. Journal of Chemical Physics, 2017, 147, 121101. | 3.0 | 13 |
| 81 | Optimized Pair Natural Orbitals for the Coupled Cluster Methods. Journal of Chemical Theory and Computation, 2018, 14, 4581-4589. | 5.3 | 13 |
| 82 | Can the distinguishable cluster approximation be improved systematically by including connected triples?. Journal of Chemical Physics, 2019, 151, . | 3.0 | 13 |
| 83 | Enabling new capabilities and insights from quantum chemistry by using component architectures. Journal of Physics: Conference Series, 2006, 46, 220-228. | 0.4 | 12 |
| 84 | A New Class of Supramolecular Wires. Journal of Physical Chemistry C, 2007, 111, 18912-18916. | 3.1 | 12 |
| 85 | Efficient evaluation of exact exchange for periodic systems via concentric atomic density fitting. Journal of Chemical Physics, 2020, 153, 124116. | 3.0 | 12 |
| 86 | 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 |
| 87 | Toward the Minimal Floating Operation Count Cholesky Decomposition of Electron Repulsion Integrals. Journal of Physical Chemistry A, 2021, 125, 4258-4265. | 2.5 | 11 |
| 88 | 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 |
| 89 | 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 |
| 90 | The elementary reaction of quartet methylidyne (CH) with methane. Molecular Physics, 1996, 89, 1695-1705. | 1.7 | 9 |

| # | Article | IF | Citations |
|---|---|---|---|
| 91 | 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 |
| 92 | Effective Utilization of Tensor Symmetry in Operation Optimization of Tensor Contraction Expressions. Procedia Computer Science, 2012, 9, 412-421. | 2.0 | 7 |
| 93 | EXAFS study of the M0.5(OH)x(H2O)yMoS2 intercalated complexes. Physica B: Condensed Matter, 1995, 208-209, 569-570. | 2.7 | 6 |
| 94 | Is F3+ viable? A high-level ab initio comparison of F3+ and Cl3+. Journal of Chemical Physics, 1998, 109, 1772-1780. | 3.0 | 6 |
| 95 | Anatomy of molecular properties evaluated with explicitly correlated electronic wave functions. Molecular Physics, 2016, 114, 2894-2909. | 1.7 | 6 |
| 96 | 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 |
| 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. Molecular Physics, 2017, 115, 2065-2076. | 1.7 | 5 |
| 99 | 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 |
| 100 | Chapter 2 Explicitly Correlated Approaches for Electronic Structure Computations. Annual Reports in Computational Chemistry, 2006, 2, 19-33. | 1.7 | 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. Physical Chemistry Chemical Physics, 2012, 14, 7863. | 2.8 | 3 |
| 103 | Spin-Free [2]<sub>R12</sub> 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 |
| 104 | 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 |
| 105 | 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 |
| 106 | Robust Pipekâ€“Mezey Orbital Localization in Periodic Solids. Journal of Chemical Theory and Computation, 2021, 17, 7406-7415. | 5.3 | 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. Journal of Statistical Physics, 2014, 154, 522-542. | 1.2 | 1 |

| # | Article | IF | Citations |
|---|---|---|---|
| 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 |
| 112 | The elementary reaction of quartet methylidyne (CH) with methane. Molecular Physics, 1996, 89, 1695-1705. | 1.7 | 0 |