# Emanuel H Rubensson

List of Publications by Year
in descending order



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|---|---|---|---|
| 30 papers | 545 citations | 623734 14 h-index | 642732 23 g-index |
| 30 all docs | 30 docs citations | 30 times ranked | 387 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Kohnâ^'Sham Density Functional Theory Electronic Structure Calculations with Linearly Scaling Computational Time and Memory Usage. Journal of Chemical Theory and Computation, 2011, 7, 340-350. | 5.3 | 88 |
| 2 | Density matrix purification with rigorous error control. Journal of Chemical Physics, 2008, 128, 074106. | 3.0 | 38 |
| 3 | Hartreeâ€"Fock calculations with linearly scaling memory usage. Journal of Chemical Physics, 2008, 128, 184106. | 3.0 | 35 |
| 4 | Systematic sparse matrix error control for linear scaling electronic structure calculations. Journal of Computational Chemistry, 2005, 26, 1628-1637. | 3.3 | 34 |
| 5 | A hierarchic sparse matrix data structure for large-scale Hartree-Fock/Kohn-Sham calculations. Journal of Computational Chemistry, 2007, 28, 2531-2537. | 3.3 | 29 |
| 6 | Graph-based linear scaling electronic structure theory. Journal of Chemical Physics, 2016, 144, 234101. | 3.0 | 29 |
| 7 | Nonmonotonic Recursive Polynomial Expansions for Linear Scaling Calculation of the Density Matrix. Journal of Chemical Theory and Computation, 2011, 7, 1233-1236. | 5.3 | 27 |
| 8 | Assessment of density matrix methods for linear scaling electronic structure calculations. Journal of Physics Condensed Matter, 2011, 23, 075502. | 1.8 | 25 |
| 9 | Bringing about matrix sparsity in linearâ€scaling electronic structure calculations. Journal of Computational Chemistry, 2011, 32, 1411-1423. | 3.3 | 24 |
| 10 | Ergo: An open-source program for linear-scaling electronic structure calculations. SoftwareX, 2018, 7, 107-111. | 2.6 | 21 |
| 11 | Interior Eigenvalues from Density Matrix Expansions in Quantum Mechanical Molecular Dynamics. SIAM Journal of Scientific Computing, 2014, 36, B147-B170. | 2.8 | 18 |
| 12 | Recursive inverse factorization. Journal of Chemical Physics, 2008, 128, 104105. | 3.0 | 17 |
| 13 | Canonical density matrix perturbation theory. Physical Review E, 2015, 92, 063301. | 2.1 | 17 |
| 14 | Chunks and Tasks: A programming model for parallelization of dynamic algorithms. Parallel Computing, 2014, 40, 328-343. | 2.1 | 16 |
| 15 | Rotations of occupied invariant subspaces in self-consistent field calculations. Journal of Mathematical Physics, 2008, 49, 032103. | 1.1 | 13 |
| 16 | Locality-aware parallel block-sparse matrix-matrix multiplication using the Chunks and Tasks programming model. Parallel Computing, 2016, 57, 87-106. | 2.1 | 13 |
| 17 | Computation of interior eigenvalues in electronic structure calculations facilitated by density matrix purification. Journal of Chemical Physics, 2008, 128, 176101. | 3.0 | 12 |
| 18 | Quantum-Based Molecular Dynamics Simulations Using Tensor Cores. Journal of Chemical Theory and Computation, 2021, 17, 6180-6192. | 5.3 | 12 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Truncation of small matrix elements based on the Euclidean norm for blocked data structures. Journal of Computational Chemistry, 2009, 30, 974-977. | 3.3 | 10 |
| 20 | Parameterless Stopping Criteria for Recursive Density Matrix Expansions. Journal of Chemical Theory and Computation, 2016, 12, 5788-5802. | 5.3 | 10 |
| 21 | A density matrix approach to the convergence of the self-consistent field iteration. Numerical Algebra, Control and Optimization, 2021, 11, 99. | 1.6 | 10 |
| 22 | Mixed Precision Fermi-Operator Expansion on Tensor Cores from a Machine Learning Perspective. Journal of Chemical Theory and Computation, 2021, 17, 2256-2265. | 5.3 | 9 |
| 23 | Controlling Errors in Recursive Fermiâ€“Dirac Operator Expansions with Applications in Electronic Structure Theory. SIAM Journal of Scientific Computing, 2012, 34, B1-B23. | 2.8 | 8 |
| 24 | Automatic Selection of Integral Thresholds by Extrapolation in Coulomb and Exchange Matrix Constructions. Journal of Chemical Theory and Computation, 2009, 5, 80-85. | 5.3 | 7 |
| 25 | Quantum Perturbation Theory Using Tensor Cores and a Deep Neural Network. Journal of Chemical Theory and Computation, 2022, 18, 4255-4268. | 5.3 | 7 |
| 26 | Linear Scaling Pseudo Fermi-Operator Expansion for Fractional Occupation. Journal of Chemical Theory and Computation, 2019, 15, 190-200. | 5.3 | 5 |
| 27 | On-the-Fly Computation of Frontal Orbitals in Density Matrix Expansions. Journal of Chemical Theory and Computation, 2018, 14, 139-153. | 5.3 | 4 |
| 28 | Localized inverse factorization. IMA Journal of Numerical Analysis, 2021, 41, 729-763. | 2.9 | 3 |
| 29 | Parallelization and scalability analysis of inverse factorization using the chunks and tasks programming model. Parallel Computing, 2019, 89, 102548. | 2.1 | 2 |
| 30 | Sparse approximate matrix-matrix multiplication for density matrix purification with error control. Journal of Computational Physics, 2021, 438, 110354. | 3.8 | 2 |