Dominika Zgid

List of Publications by Year
in descending order

40	1,872	218677	289244
papers	citations	26 h-index	40 g-index

40	40	40	1124
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Towards the Solution of the Many-Electron Problem in Real Materials: Equation of State of the Hydrogen Chain with State-of-the-Art Many-Body Methods. Physical Review X, 2017, 7, .	8.9	171
2	The density matrix renormalization group self-consistent field method: Orbital optimization with the density matrix renormalization group method in the active space. Journal of Chemical Physics, 2008, 128, 144116.	3.0	164
3	Truncated configuration interaction expansions as solvers for correlated quantum impurity models and dynamical mean-field theory. Physical Review B, 2012, 86, .	3.2	107
4	Dynamical mean-field theory from a quantum chemical perspective. Journal of Chemical Physics, 2011, 134, 094115.	3.0	106
5	Communication: The description of strong correlation within self-consistent Green's function second-order perturbation theory. Journal of Chemical Physics, 2014, 140, 241101.	3.0	87
6	Obtaining the two-body density matrix in the density matrix renormalization group method. Journal of Chemical Physics, 2008, 128, 144115.	3.0	81
7	Systematically improvable multiscale solver for correlated electron systems. Physical Review B, 2015, 91, .	3.2	77
8	Communication: Towards ab initio self-energy embedding theory in quantum chemistry. Journal of Chemical Physics, 2015, 143, 241102.	3.0	76
9	Self-consistent second-order Greenâ€™s function perturbation theory for periodic systems. Journal of Chemical Physics, 2016, 144, 054106.	3.0	75
10	Chapter 7 The Density Matrix Renormalization Group in Quantum Chemistry. Annual Reports in Computational Chemistry, 2009, 5, 149-162.	1.7	72
11	A study of cumulant approximations to n-electron valence multireference perturbation theory. Journal of Chemical Physics, 2009, 130, 194107.	3.0	70
12	Direct Comparison of Many-Body Methods for Realistic Electronic Hamiltonians. Physical Review X, 2020, 10, .	8.9	68
13	Finite temperature quantum embedding theories for correlated systems. New Journal of Physics, 2017, 19, 023047.	2.9	63
14	Self-Energy Embedding Theory (SEET) for Periodic Systems. Journal of Chemical Theory and Computation, 2019, 15, 229-240.	5.3	47
15	Generalized Self-Energy Embedding Theory. Journal of Physical Chemistry Letters, 2017, 8, 2200-2205.	4.6	45
16	Rigorous Ab Initio Quantum Embedding for Quantum Chemistry Using Greenâ€™s Function Theory: Screened Interaction, Nonlocal Self-Energy Relaxation, Orbital Basis, and Chemical Accuracy. Journal of Chemical Theory and Computation, 2016, 12, 4856-4870.	5.3	44
17	Exploring connections between statistical mechanics and Greenâ€™s functions for realistic systems: Temperature dependent electronic entropy and internal energy from a self-consistent second-order Greenâ€™s function. Journal of Chemical Physics, 2016, 145, 204106.	3.0	43
18	Efficient Temperature-Dependent Greenâ€™s Functions Methods for Realistic Systems: Compact Grids for Orthogonal Polynomial Transforms. Journal of Chemical Theory and Computation, 2016, 12, 564-571.	5.3	40

#	Article	IF	Citations
19	Stochastic Self-Consistent Second-Order Greenâ€™s Function Method for Correlation Energies of Large Electronic Systems. Journal of Chemical Theory and Computation, 2017, 13, 5396-5403.	5.3	40
20	Fractional charge and spin errors in self-consistent Greenâ€™s function theory. Journal of Chemical Physics, 2015, 142, 194108.	3.0	37
21	Local Hamiltonians for quantitative Green's function embedding methods. Journal of Chemical Physics, 2014, 141, 194105.	3.0	34
22	Coupled Cluster as an Impurity Solver for Greenâ€™s Function Embedding Methods. Journal of Chemical Theory and Computation, 2019, 15, 6010-6024.	5.3	34
23	Chebyshev polynomial representation of imaginary-time response functions. Physical Review B, 2018, 98, .	3.2	32
24	Ab initio self-energy embedding for the photoemission spectra of NiO and MnO. Physical Review B, 2020, 102, .	3.2	31
25	Analytical continuation of matrix-valued functions: CarathÃ©odory formalism. Physical Review B, 2021, 104, .	3.2	31
26	Efficient Temperature-Dependent Greenâ€™s Function Methods for Realistic Systems: Using Cubic Spline Interpolation to Approximate Matsubara Greenâ€™s Functions. Journal of Chemical Theory and Computation, 2016, 12, 2250-2259.	5.3	30
27	Testing self-energy embedding theory in combination with GW. Physical Review B, 2017, 96, .	3.2	22
28	Effect of propagator renormalization on the band gap of insulating solids. Physical Review B, 2019, 100, .	3.2	19
29	Legendre-spectral Dyson equation solver with super-exponential convergence. Journal of Chemical Physics, 2020, 152, 134107.	3.0	19
30	Spin-Unrestricted Self-Energy Embedding Theory. Journal of Physical Chemistry Letters, 2018, 9, 4444-4450.	4.6	17
31	Interpretation of multiple solutions in fully iterative GF2 and GW schemes using local analysis of two-particle density matrices. Journal of Chemical Physics, 2021, 155, 024101.	3.0	17
32	Evaluation of two-particle properties within finite-temperature self-consistent one-particle Greenâ€™s function methods: Theory and application to GW and GF2. Journal of Chemical Physics, 2021, 155, 024119.	3.0	16
33	Electron correlations in the cubic paramagnetic perovskite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Sr</mml:mi><mml:mo>(</mml:mo><mml:mi) Tj ETQq1 1 0.784314 g mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> : Results from fully self-consistent self-energy embedding calculations. Physical Review B, 2021, 103, .	3.2	13
34	Iterative subspace algorithms for finite-temperature solution of Dyson equation. Journal of Chemical Physics, 2022, 156, 094101.	3.0	11
35	Combining Density Functional Theory and Greenâ€™s Function Theory: Range-Separated, Nonlocal, Dynamic, and Orbital-Dependent Hybrid Functional. Journal of Chemical Theory and Computation, 2017, 13, 5317-5331.	5.3	10
36	Testing the Green's function coupled cluster singles and doubles impurity solver on real materials within the framework of self-energy embedding theory. Physical Review B, 2021, 103, .	3.2	8

#	Article	IF	Citations
37	Exploring Coupled Cluster Greenâ€™s Function as a Method for Treating System and Environment in Greenâ€™s Function Embedding Methods. Journal of Chemical Theory and Computation, 2022, 18, 664-676.	5.3	7
38	Material-Specific Optimization of Gaussian Basis Sets against Plane Wave Data. Journal of Chemical Theory and Computation, 2021, 17, 5611-5622.	5.3	6
39	Sparse-Hamiltonian approach to the time-evolution of molecules on quantum computers. European Physical Journal: Special Topics, 2021, 230, 1067-1071.	2.6	1
40	Dynamical Self-energy Mapping (DSEM) for Creation of Sparse Hamiltonians Suitable for Quantum Computing. Journal of Chemical Theory and Computation, 2021, , .	5.3	1