Anders M N Niklasson

List of Publications by Year
in descending order

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76 papers	3,240 citations	172457 29 h-index	149698 56 g-index
77 all docs	77 docs citations	77 times ranked	2309 citing authors

#	Article	IF	Citations
1	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. Journal of Chemical Physics, 2020, 152, 124101.	3.0	589
2	Order-NGreen's Function Technique for Local Environment Effects in Alloys. Physical Review Letters, 1996, 76, 4203-4206.	7.8	210
3	Time-Reversible Born-Oppenheimer Molecular Dynamics. Physical Review Letters, 2006, 97, 123001.	7.8	132
4	Extended Born-Oppenheimer Molecular Dynamics. Physical Review Letters, 2008, 100, 123004.	7.8	130
5	Expansion algorithm for the density matrix. Physical Review B, 2002, 66, .	3.2	120
6	Interface magnetism of3dtransition metals. Physical Review B, 1999, 59, 6373-6382.	3.2	115
7	Extended Lagrangian Bornâ€“Oppenheimer molecular dynamics with dissipation. Journal of Chemical Physics, 2009, 130, 214109.	3.0	114
8	Trace resetting density matrix purification in O(N) self-consistent-field theory. Journal of Chemical Physics, 2003, 118, 8611-8620.	3.0	95
9	Representation independent algorithms for molecular response calculations in time-dependent self-consistent field theories. Journal of Chemical Physics, 2009, 130, 054111.	3.0	92
10	Orbital Magnetism and Magnetic Anisotropy Probed with Ferromagnetic Resonance. Physical Review Letters, 1999, 82, 2390-2393.	7.8	87
11	Density Matrix Perturbation Theory. Physical Review Letters, 2004, 92, 193001.	7.8	71
12	Calculated oscillation periods of the interlayer coupling in Fe/Cr/Fe and Fe/Mo/Fe sandwiches. Physical Review B, 1996, 54, 6382-6392.	3.2	63
13	Lagrangian formulation with dissipation of Born-Oppenheimer molecular dynamics using the density-functional tight-binding method. Journal of Chemical Physics, 2011, 135, 044122.	3.0	63
14	Energy conserving, linear scaling Born-Oppenheimer molecular dynamics. Journal of Chemical Physics, 2012, 137, 134105.	3.0	61
15	Wave function extended Lagrangian Born-Oppenheimer molecular dynamics. Physical Review B, 2010, 82, .	3.2	59
16	Direct energy functional minimization under orthogonality constraints. Journal of Chemical Physics, 2008, 128, 084113.	3.0	52
17	Ab InitioLinear Scaling Response Theory: Electric Polarizability by Perturbed Projection. Physical Review Letters, 2004, 92, 193002.	7.8	49
18	Spin Density Waves in Thin Chromium Films. Physical Review Letters, 1999, 82, 4544-4547.	7.8	46

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19	Generalized extended Lagrangian Born-Oppenheimer molecular dynamics. Journal of Chemical Physics, 2014, 141, 164123.	3.0	45
20	Time-reversible ab initio molecular dynamics. Journal of Chemical Physics, 2007, 126, 144103.	3.0	44
21	Sample Preserving Deep Interface Characterization Technique. Physical Review Letters, 2006, 97, 266106.	7.8	38
22	Accurate Classical Polarization Solution with No Self-Consistent Field Iterations. Journal of Physical Chemistry Letters, 2017, 8, 1714-1723.	4.6	38
23	Quantum-well-induced ferromagnetism in thin films. Physical Review B, 1997, 56, 3276-3280.	3.2	36
24	Implicit purification for temperature-dependent density matrices. Physical Review B, 2003, 68, .	3.2	36
25	Higher-order symplectic integration in Bornâ€“Oppenheimer molecular dynamics. Journal of Chemical Physics, 2009, 131, 244106.	3.0	33
26	First principles molecular dynamics without self-consistent field optimization. Journal of Chemical Physics, 2014, 140, 044117.	3.0	33
27	Numerical Optimization of Density Functional Tight Binding Models: Application to Molecules Containing Carbon, Hydrogen, Nitrogen, and Oxygen. Journal of Chemical Theory and Computation, 2017, 13, 6191-6200.	5.3	33
28	A note on the Pulay force at finite electronic temperatures. Journal of Chemical Physics, 2008, 129, 244107.	3.0	32
29	Iterative refinement method for the approximate factorization of a matrix inverse. Physical Review B, 2004, 70, .	3.2	29
30	Graph-based linear scaling electronic structure theory. Journal of Chemical Physics, 2016, 144, 234101.	3.0	29
31	Multiple-scattering theoretical approach to magnetic dichroism and spin polarization in angle-resolved core-level photoemission. Physical Review B, 1999, 59, 13986-14000.	3.2	28
32	Next generation extended Lagrangian first principles molecular dynamics. Journal of Chemical Physics, 2017, 147, 054103.	3.0	27
33	Extended Lagrangian Density Functional Tight-Binding Molecular Dynamics for Molecules and Solids. Journal of Chemical Theory and Computation, 2015, 11, 3357-3363.	5.3	26
34	Extended Lagrangian Born-Oppenheimer molecular dynamics simulations of the shock-induced chemistry of phenylacetylene. Journal of Chemical Physics, 2015, 142, 064512.	3.0	26
35	Performance of extended Lagrangian schemes for molecular dynamics simulations with classical polarizable force fields and density functional theory. Journal of Chemical Physics, 2017, 146, 124115.	3.0	26
36	Thermostating extended Lagrangian Born-Oppenheimer molecular dynamics. Journal of Chemical Physics, 2015, 142, 154120.	3.0	25

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37	Linear scaling density matrix perturbation theory for basis-set-dependent quantum response calculations: An orthogonal formulation. Journal of Chemical Physics, 2007, 127, 064105.	3.0	24
38	Graphics Processing Unit-Accelerated Semiempirical Born Oppenheimer Molecular Dynamics Using PyTorch. Journal of Chemical Theory and Computation, 2020, 16, 4951-4962.	5.3	24
39	Efficient Parallel Linear Scaling Construction of the Density Matrix for Bornâ€“Oppenheimer Molecular Dynamics. Journal of Chemical Theory and Computation, 2015, 11, 4644-4654.	5.3	23
40	Magnetism and anisotropy of ultrathin Ni films on Cu(001). Physical Review B, 1999, 59, 9332-9341.	3.2	22
41	Higher-order response in O(N) by perturbed projection. Journal of Chemical Physics, 2005, 123, 044106.	3.0	22
42	Nonorthogonal density-matrix perturbation theory. Journal of Chemical Physics, 2005, 123, 044107.	3.0	21
43	Fast method for quantum mechanical molecular dynamics. Physical Review B, 2012, 86, .	3.2	21
44	Extended Lagrangian free energy molecular dynamics. Journal of Chemical Physics, 2011, 135, 164111.	3.0	19
45	Geometric integration in Born-Oppenheimer molecular dynamics. Journal of Chemical Physics, 2011, 135, 224105.	3.0	19
46	Computing the Density Matrix in Electronic Structure Theory on Graphics Processing Units. Journal of Chemical Theory and Computation, 2012, 8, 4094-4101.	5.3	19
47	Recursive Factorization of the Inverse Overlap Matrix in Linear-Scaling Quantum Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2016, 12, 3063-3073.	5.3	19
48	Quantum-well states and induced magnetism in Fe/CuN/Fe bcc (001) trilayers. Physical Review B, 1996, 53, 8509-8514.	3.2	18
49	Interior Eigenvalues from Density Matrix Expansions in Quantum Mechanical Molecular Dynamics. SIAM Journal of Scientific Computing, 2014, 36, B147-B170.	2.8	18
50	Recursive inverse factorization. Journal of Chemical Physics, 2008, 128, 104105.	3.0	17
51	Canonical density matrix perturbation theory. Physical Review E, 2015, 92, 063301.	2.1	17
52	Molecular-orbital-free algorithm for excited states in time-dependent perturbation theory. Journal of Chemical Physics, 2008, 129, 064114.	3.0	16
53	Extended Lagrangian Born-Oppenheimer molecular dynamics in the limit of vanishing self-consistent field optimization. Journal of Chemical Physics, 2013, 139, 214102.	3.0	16
54	The Middle Science: Traversing Scale In Complex Many-Body Systems. ACS Central Science, 2021, 7, 1271-1287.	11.3	16

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55	Extended Lagrangian Bornâ€“Oppenheimer molecular dynamics using a Krylov subspace approximation. Journal of Chemical Physics, 2020, 152, 104103.	3.0	15
56	Higher-Order Extended Lagrangian Bornâ€“Oppenheimer Molecular Dynamics for Classical Polarizable Models. Journal of Chemical Theory and Computation, 2018, 14, 499-511.	5.3	12
57	The basic matrix library (BML) for quantum chemistry. Journal of Supercomputing, 2018, 74, 6201-6219.	3.6	12
58	Quantum-Based Molecular Dynamics Simulations Using Tensor Cores. Journal of Chemical Theory and Computation, 2021, 17, 6180-6192.	5.3	12
59	Computation of the Density Matrix in Electronic Structure Theory in Parallel on Multiple Graphics Processing Units. Journal of Chemical Theory and Computation, 2014, 10, 5391-5396.	5.3	10
60	Density-Matrix Based Extended Lagrangian Bornâ€“Oppenheimer Molecular Dynamics. Journal of Chemical Theory and Computation, 2020, 16, 3628-3640.	5.3	10
61	Interface mixing energy: A measure of interface stability. Physical Review B, 1998, 58, 3613-3616.	3.2	9
62	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
63	Extended Lagrangian Excited State Molecular Dynamics. Journal of Chemical Theory and Computation, 2018, 14, 799-806.	5.3	8
64	Observation of short- and long-range hybridization of a buried Cu monolayer in Ni. Physical Review B, 2000, 62, R16239-R16242.	3.2	7
65	Using Graph Partitioning for Scalable Distributed Quantum Molecular Dynamics. Algorithms, 2019, 12, 187.	2.1	7
66	Quantum Perturbation Theory Using Tensor Cores and a Deep Neural Network. Journal of Chemical Theory and Computation, 2022, 18, 4255-4268.	5.3	7
67	Extended Lagrangian Bornâ€“Oppenheimer molecular dynamics for orbital-free density-functional theory and polarizable charge equilibration models. Journal of Chemical Physics, 2021, 154, 054101.	3.0	6
68	Extended Lagrangian Bornâ€“Oppenheimer molecular dynamics: from density functional theory to charge relaxation models. European Physical Journal B, 2021, 94, 1.	1.5	6
69	Linear Scaling Pseudo Fermi-Operator Expansion for Fractional Occupation. Journal of Chemical Theory and Computation, 2019, 15, 190-200.	5.3	5
70	Magnetic interlayer coupling and interaction between interface states in a quantum-well system. Journal of Physics Condensed Matter, 1999, 11, 975-988.	1.8	4
71	Density Matrix Methods in Linear Scaling Electronic Structure Theory. Challenges and Advances in Computational Chemistry and Physics, 2011, , 439-473.	0.6	4
72	Trace correcting density matrix extrapolation in self-consistent geometry optimization. Journal of Chemical Physics, 2010, 132, 124104.	3.0	3

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73	Extended Lagrangian Formulation of Charge-Constrained Tight-Binding Molecular Dynamics. Journal of Chemical Theory and Computation, 2015, 11, 2697-2704.	5.3	2
74	Shadow Lagrangian dynamics for superfluidity. Kinetic and Related Models, 2021, 14, 303.	0.9	2
75	Quantum-Based Molecular Dynamics Simulations with Applications to Industrial Problems. Springer Series in Materials Science, 2021, , 289-314.	0.6	2
76	Magnetic structure and anisotropy of ultra-thin Ni films on Cu(001). The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1998, 78, 585-589.	0.6	1