

Gustavo E Scuseria

List of Publications by Year in descending order

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Version: 2024-02-01

393
papers

62,669
citations

4120

87
h-index

813

246
g-index

400
all docs

400
docs citations

400
times ranked

33901
citing authors

#	ARTICLE	IF	CITATIONS
1	Thermal coupled cluster theory for SU(2) systems. <i>Physical Review B</i> , 2022, 105, .	1.1	5
2	A power series approximation in symmetry projected coupled cluster theory. <i>Journal of Chemical Physics</i> , 2022, 156, 104105.	1.2	3
3	Coupled Cluster and Perturbation Theories Based on a Cluster Mean-Field Reference Applied to Strongly Correlated Spin Systems. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4293-4303.	2.3	8
4	Confronting Racism in Chemistry Journals. <i>ACS ES&T Engineering</i> , 2021, 1, 3-5.	3.7	0
5	Confronting Racism in Chemistry Journals. <i>ACS ES&T Water</i> , 2021, 1, 3-5.	2.3	0
6	Exploring non-linear correlators on AGP. <i>Journal of Chemical Physics</i> , 2021, 154, 074113.	1.2	26
7	Construction of linearly independent non-orthogonal AGP states. <i>Journal of Chemical Physics</i> , 2021, 154, 114112.	1.2	15
8	Advancing solid-state band gap predictions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	3
9	Correlating AGP on a quantum computer. <i>Quantum Science and Technology</i> , 2021, 6, 014004.	2.6	37
10	Assessing combinations of singlet-paired coupled cluster and density functional theory for treating electron correlation in closed and open shells. <i>Molecular Physics</i> , 2020, 118, 1615144.	0.8	1
11	Confronting Racism in Chemistry Journals. <i>ACS Pharmacology and Translational Science</i> , 2020, 3, 559-561.	2.5	0
12	Confronting Racism in Chemistry Journals. <i>Biochemistry</i> , 2020, 59, 2313-2315.	1.2	0
13	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. <i>ACS Biomaterials Science and Engineering</i> , 2020, 6, 2707-2708.	2.6	0
14	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. <i>ACS Central Science</i> , 2020, 6, 589-590.	5.3	0
15	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. <i>ACS Chemical Biology</i> , 2020, 15, 1282-1283.	1.6	0
16	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. <i>ACS Chemical Neuroscience</i> , 2020, 11, 1196-1197.	1.7	0
17	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. <i>ACS Earth and Space Chemistry</i> , 2020, 4, 672-673.	1.2	0
18	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. <i>ACS Energy Letters</i> , 2020, 5, 1610-1611.	8.8	1

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19	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. ACS Macro Letters, 2020, 9, 666-667.	2.3	0
20	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. , 2020, 2, 563-564.		0
21	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. ACS Nano, 2020, 14, 5151-5152.	7.3	2
22	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. ACS Photonics, 2020, 7, 1080-1081.	3.2	0
23	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. ACS Pharmacology and Translational Science, 2020, 3, 455-456.	2.5	0
24	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. ACS Sustainable Chemistry and Engineering, 2020, 8, 6574-6575.	3.2	0
25	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Analytical Chemistry, 2020, 92, 6187-6188.	3.2	0
26	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Chemistry of Materials, 2020, 32, 3678-3679.	3.2	0
27	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Environmental Science and Technology Letters, 2020, 7, 280-281.	3.9	1
28	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Journal of Chemical Education, 2020, 97, 1217-1218.	1.1	1
29	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Journal of Proteome Research, 2020, 19, 1883-1884.	1.8	0
30	Confronting Racism in Chemistry Journals. Langmuir, 2020, 36, 7155-7157.	1.6	0
31	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. ACS Applied Polymer Materials, 2020, 2, 1739-1740.	2.0	0
32	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. ACS Combinatorial Science, 2020, 22, 223-224.	3.8	0
33	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. ACS Medicinal Chemistry Letters, 2020, 11, 1060-1061.	1.3	0
34	Wave function methods for canonical ensemble thermal averages in correlated many-fermion systems. Journal of Chemical Physics, 2020, 153, 124115.	1.2	15
35	Editorial Confronting Racism in Chemistry Journals. , 2020, 2, 829-831.		0
36	Confronting Racism in Chemistry Journals. Journal of Physical Chemistry Letters, 2020, 11, 5279-5281.	2.1	1

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37	Confronting Racism in Chemistry Journals. ACS Applied Energy Materials, 2020, 3, 6016-6018.	2.5	0
38	Confronting Racism in Chemistry Journals. ACS Central Science, 2020, 6, 1012-1014.	5.3	1
39	Confronting Racism in Chemistry Journals. Industrial & Engineering Chemistry Research, 2020, 59, 11915-11917.	1.8	0
40	Confronting Racism in Chemistry Journals. Journal of Natural Products, 2020, 83, 2057-2059.	1.5	0
41	Confronting Racism in Chemistry Journals. ACS Medicinal Chemistry Letters, 2020, 11, 1354-1356.	1.3	0
42	Confronting Racism in Chemistry Journals. Journal of the American Society for Mass Spectrometry, 2020, 31, 1321-1323.	1.2	1
43	Confronting Racism in Chemistry Journals. Energy & Fuels, 2020, 34, 7771-7773.	2.5	0
44	Confronting Racism in Chemistry Journals. ACS Sensors, 2020, 5, 1858-1860.	4.0	0
45	Geminal Replacement Models Based on AGP. Journal of Chemical Theory and Computation, 2020, 16, 6358-6367.	2.3	22
46	Confronting Racism in Chemistry Journals. ACS Nano, 2020, 14, 7675-7677.	7.3	2
47	Correlating the antisymmetrized geminal power wave function. Journal of Chemical Physics, 2020, 153, 084111.	1.2	28
48	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Biochemistry, 2020, 59, 1641-1642.	1.2	0
49	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Journal of Chemical & Engineering Data, 2020, 65, 2253-2254.	1.0	0
50	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Organic Process Research and Development, 2020, 24, 872-873.	1.3	0
51	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. ACS Omega, 2020, 5, 9624-9625.	1.6	0
52	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. ACS Applied Electronic Materials, 2020, 2, 1184-1185.	2.0	0
53	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. ACS Applied Materials & Interfaces, 2020, 12, 20147-20148.	4.0	5
54	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Journal of Physical Chemistry C, 2020, 124, 9629-9630.	1.5	0

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55	Update to Our Reader, Reviewer, and Author Communities" April 2020. Journal of Physical Chemistry Letters, 2020, 11, 3571-3572.	2.1	0
56	Update to Our Reader, Reviewer, and Author Communities" April 2020. ACS Synthetic Biology, 2020, 9, 979-980.	1.9	0
57	Update to Our Reader, Reviewer, and Author Communities" April 2020. ACS Applied Energy Materials, 2020, 3, 4091-4092.	2.5	0
58	Confronting Racism in Chemistry Journals. Journal of Chemical Theory and Computation, 2020, 16, 4003-4005.	2.3	0
59	Confronting Racism in Chemistry Journals. Journal of Organic Chemistry, 2020, 85, 8297-8299.	1.7	0
60	Confronting Racism in Chemistry Journals. Analytical Chemistry, 2020, 92, 8625-8627.	3.2	0
61	Confronting Racism in Chemistry Journals. Journal of Chemical Education, 2020, 97, 1695-1697.	1.1	0
62	Confronting Racism in Chemistry Journals. Organic Process Research and Development, 2020, 24, 1215-1217.	1.3	0
63	Confronting Racism in Chemistry Journals. ACS Sustainable Chemistry and Engineering, 2020, 8, .	3.2	0
64	Confronting Racism in Chemistry Journals. Chemistry of Materials, 2020, 32, 5369-5371.	3.2	0
65	Confronting Racism in Chemistry Journals. Chemical Research in Toxicology, 2020, 33, 1511-1513.	1.7	0
66	Confronting Racism in Chemistry Journals. Inorganic Chemistry, 2020, 59, 8639-8641.	1.9	0
67	Confronting Racism in Chemistry Journals. ACS Applied Nano Materials, 2020, 3, 6131-6133.	2.4	0
68	Confronting Racism in Chemistry Journals. ACS Applied Polymer Materials, 2020, 2, 2496-2498.	2.0	0
69	Confronting Racism in Chemistry Journals. ACS Chemical Biology, 2020, 15, 1719-1721.	1.6	0
70	Update to Our Reader, Reviewer, and Author Communities" April 2020. Journal of Chemical Theory and Computation, 2020, 16, 2881-2882.	2.3	0
71	Confronting Racism in Chemistry Journals. Organic Letters, 2020, 22, 4919-4921.	2.4	4
72	Confronting Racism in Chemistry Journals. ACS Applied Materials & Interfaces, 2020, 12, 28925-28927.	4.0	13

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73	Confronting Racism in Chemistry Journals. <i>Crystal Growth and Design</i> , 2020, 20, 4201-4203.	1.4	1
74	Confronting Racism in Chemistry Journals. <i>Chemical Reviews</i> , 2020, 120, 5795-5797.	23.0	2
75	Confronting Racism in Chemistry Journals. <i>ACS Catalysis</i> , 2020, 10, 7307-7309.	5.5	1
76	Confronting Racism in Chemistry Journals. <i>Biomacromolecules</i> , 2020, 21, 2543-2545.	2.6	0
77	Confronting Racism in Chemistry Journals. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 6575-6577.	2.9	0
78	Confronting Racism in Chemistry Journals. <i>Macromolecules</i> , 2020, 53, 5015-5017.	2.2	0
79	Confronting Racism in Chemistry Journals. <i>Nano Letters</i> , 2020, 20, 4715-4717.	4.5	5
80	Confronting Racism in Chemistry Journals. <i>Organometallics</i> , 2020, 39, 2331-2333.	1.1	0
81	Confronting Racism in Chemistry Journals. <i>Journal of the American Chemical Society</i> , 2020, 142, 11319-11321.	6.6	1
82	Confronting Racism in Chemistry Journals. <i>Accounts of Chemical Research</i> , 2020, 53, 1257-1259.	7.6	0
83	Confronting Racism in Chemistry Journals. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5271-5273.	1.1	0
84	Confronting Racism in Chemistry Journals. <i>ACS Energy Letters</i> , 2020, 5, 2291-2293.	8.8	0
85	Confronting Racism in Chemistry Journals. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3325-3327.	2.5	0
86	Confronting Racism in Chemistry Journals. <i>Journal of Proteome Research</i> , 2020, 19, 2911-2913.	1.8	0
87	Confronting Racism in Chemistry Journals. <i>Journal of Physical Chemistry B</i> , 2020, 124, 5335-5337.	1.2	1
88	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. <i>Journal of Agricultural and Food Chemistry</i> , 2020, 68, 5019-5020.	2.4	0
89	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. <i>Journal of Physical Chemistry B</i> , 2020, 124, 3603-3604.	1.2	0
90	Confronting Racism in Chemistry Journals. <i>Bioconjugate Chemistry</i> , 2020, 31, 1693-1695.	1.8	0

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91	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. ACS Applied Nano Materials, 2020, 3, 3960-3961.	2.4	0
92	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Journal of Natural Products, 2020, 83, 1357-1358.	1.5	0
93	Confronting Racism in Chemistry Journals. ACS Synthetic Biology, 2020, 9, 1487-1489.	1.9	0
94	Confronting Racism in Chemistry Journals. Journal of Chemical & Engineering Data, 2020, 65, 3403-3405.	1.0	0
95	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Bioconjugate Chemistry, 2020, 31, 1211-1212.	1.8	0
96	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Journal of Chemical Health and Safety, 2020, 27, 133-134.	1.1	0
97	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Chemical Research in Toxicology, 2020, 33, 1509-1510.	1.7	0
98	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Energy & Fuels, 2020, 34, 5107-5108.	2.5	0
99	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. ACS Applied Bio Materials, 2020, 3, 2873-2874.	2.3	0
100	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Journal of Organic Chemistry, 2020, 85, 5751-5752.	1.7	0
101	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Journal of the American Society for Mass Spectrometry, 2020, 31, 1006-1007.	1.2	0
102	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Accounts of Chemical Research, 2020, 53, 1001-1002.	7.6	0
103	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Biomacromolecules, 2020, 21, 1966-1967.	2.6	0
104	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Chemical Reviews, 2020, 120, 3939-3940.	23.0	0
105	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Environmental Science & Technology, 2020, 54, 5307-5308.	4.6	0
106	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Langmuir, 2020, 36, 4565-4566.	1.6	0
107	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Molecular Pharmaceutics, 2020, 17, 1445-1446.	2.3	0
108	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. ACS Infectious Diseases, 2020, 6, 891-892.	1.8	0

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109	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Crystal Growth and Design, 2020, 20, 2817-2818.	1.4	1
110	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Journal of Medicinal Chemistry, 2020, 63, 4409-4410.	2.9	0
111	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Journal of Physical Chemistry A, 2020, 124, 3501-3502.	1.1	0
112	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Nano Letters, 2020, 20, 2935-2936.	4.5	0
113	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. ACS Sensors, 2020, 5, 1251-1252.	4.0	0
114	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Journal of Chemical Information and Modeling, 2020, 60, 2651-2652.	2.5	0
115	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Industrial & Engineering Chemistry Research, 2020, 59, 8509-8510.	1.8	0
116	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Journal of the American Chemical Society, 2020, 142, 8059-8060.	6.6	3
117	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Inorganic Chemistry, 2020, 59, 5796-5797.	1.9	0
118	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Organometallics, 2020, 39, 1665-1666.	1.1	0
119	Update to Our Reader, Reviewer, and Author Communitiesâ€™ April 2020. Organic Letters, 2020, 22, 3307-3308.	2.4	0
120	Confronting Racism in Chemistry Journals. ACS Biomaterials Science and Engineering, 2020, 6, 3690-3692.	2.6	1
121	Confronting Racism in Chemistry Journals. ACS Omega, 2020, 5, 14857-14859.	1.6	1
122	Confronting Racism in Chemistry Journals. ACS Applied Electronic Materials, 2020, 2, 1774-1776.	2.0	0
123	Confronting Racism in Chemistry Journals. Journal of Agricultural and Food Chemistry, 2020, 68, 6941-6943.	2.4	0
124	Confronting Racism in Chemistry Journals. ACS Earth and Space Chemistry, 2020, 4, 961-963.	1.2	0
125	Confronting Racism in Chemistry Journals. Environmental Science and Technology Letters, 2020, 7, 447-449.	3.9	0
126	Confronting Racism in Chemistry Journals. ACS Combinatorial Science, 2020, 22, 327-329.	3.8	0

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127	Confronting Racism in Chemistry Journals. ACS Infectious Diseases, 2020, 6, 1529-1531.	1.8	0
128	Confronting Racism in Chemistry Journals. ACS Applied Bio Materials, 2020, 3, 3925-3927.	2.3	0
129	Confronting Racism in Chemistry Journals. Journal of Physical Chemistry C, 2020, 124, 14069-14071.	1.5	0
130	Confronting Racism in Chemistry Journals. ACS Macro Letters, 2020, 9, 1004-1006.	2.3	0
131	Confronting Racism in Chemistry Journals. Molecular Pharmaceutics, 2020, 17, 2229-2231.	2.3	1
132	Confronting Racism in Chemistry Journals. ACS Chemical Neuroscience, 2020, 11, 1852-1854.	1.7	1
133	Confronting Racism in Chemistry Journals. ACS Photonics, 2020, 7, 1586-1588.	3.2	0
134	Confronting Racism in Chemistry Journals. Environmental Science & Technology, 2020, 54, 7735-7737.	4.6	0
135	Confronting Racism in Chemistry Journals. Journal of Chemical Health and Safety, 2020, 27, 198-200.	1.1	0
136	Geminal-based configuration interaction. Journal of Chemical Physics, 2019, 151, .	1.2	31
137	Thermofield Theory for Finite-Temperature Coupled Cluster. Journal of Chemical Theory and Computation, 2019, 15, 6127-6136.	2.3	30
138	Thermofield theory for finite-temperature quantum chemistry. Journal of Chemical Physics, 2019, 150, 154109.	1.2	30
139	Polynomial-product states: A symmetry-projection-based factorization of the full coupled cluster wavefunction in terms of polynomials of double excitations. Journal of Chemical Physics, 2019, 150, 144108.	1.2	9
140	Efficient evaluation of AGP reduced density matrices. Journal of Chemical Physics, 2019, 151, 184103.	1.2	26
141	Exact parameterization of fermionic wave functions via unitary coupled cluster theory. Journal of Chemical Physics, 2019, 151, 244112.	1.2	124
142	On the difference between variational and unitary coupled cluster theories. Journal of Chemical Physics, 2018, 148, 044107.	1.2	70
143	Hartree-Fock symmetry breaking around conical intersections. Journal of Chemical Physics, 2018, 148, 024109.	1.2	11
144	Influence of broken-pair excitations on the exact pair wavefunction. Molecular Physics, 2018, 116, 186-193.	0.8	8

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145	Magnetic Structure of Density Matrices. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 649-659.	2.3	12
146	Projected coupled cluster theory: Optimization of cluster amplitudes in the presence of symmetry projection. <i>Journal of Chemical Physics</i> , 2018, 149, 164108.	1.2	18
147	Assessment of the Tao-Mo nonempirical semilocal density functional in applications to solids and surfaces. <i>Physical Review B</i> , 2017, 95, .	1.1	37
148	Merging symmetry projection methods with coupled cluster theory: Lessons from the Lipkin model Hamiltonian. <i>Journal of Chemical Physics</i> , 2017, 146, 054110.	1.2	30
149	Understanding band gaps of solids in generalized Kohn-Sham theory. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 2801-2806.	3.3	423
150	Projected Hartree-Fock theory as a polynomial of particle-hole excitations and its combination with variational coupled cluster theory. <i>Journal of Chemical Physics</i> , 2017, 146, 184105.	1.2	22
151	Semilocal exchange hole with an application to range-separated density functionals. <i>Physical Review B</i> , 2017, 95, .	1.1	19
152	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. <i>Physical Review X</i> , 2017, 7, .	2.8	171
153	Spin-projected generalized Hartree-Fock method as a polynomial of particle-hole excitations. <i>Physical Review A</i> , 2017, 96, .	1.0	11
154	Combining symmetry collective states with coupled-cluster theory: Lessons from the Agassi model Hamiltonian. <i>Physical Review C</i> , 2017, 95, .	1.1	11
155	Projected coupled cluster theory. <i>Journal of Chemical Physics</i> , 2017, 147, 064111.	1.2	56
156	Electronic Structure and Properties of Berkelium Iodates. <i>Journal of the American Chemical Society</i> , 2017, 139, 13361-13375.	6.6	25
157	Attenuated coupled cluster: a heuristic polynomial similarity transformation incorporating spin symmetry projection into traditional coupled cluster theory. <i>Molecular Physics</i> , 2017, 115, 2673-2683.	0.8	11
158	Spin polynomial similarity transformation for repulsive Hamiltonians: interpolating between coupled cluster and spin-projected unrestricted Hartree-Fock. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 22385-22394.	1.3	4
159	Tensor-structured coupled cluster theory. <i>Journal of Chemical Physics</i> , 2017, 147, 184113.	1.2	48
160	Recoupling the singlet- and triplet-pairing channels in single-reference coupled cluster theory. <i>Journal of Chemical Physics</i> , 2016, 145, 134103.	1.2	13
161	Blind test of density-functional-based methods on intermolecular interaction energies. <i>Journal of Chemical Physics</i> , 2016, 145, 124105.	1.2	97
162	Singlet-paired coupled cluster theory for open shells. <i>Journal of Chemical Physics</i> , 2016, 144, 244117.	1.2	19

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163	Using full configuration interaction quantum Monte Carlo in a seniority zero space to investigate the correlation energy equivalence of pair coupled cluster doubles and doubly occupied configuration interaction. <i>Journal of Chemical Physics</i> , 2016, 144, 094112.	1.2	26
164	Performance of a nonempirical density functional on molecules and hydrogen-bonded complexes. <i>Journal of Chemical Physics</i> , 2016, 145, 234306.	1.2	25
165	Predicting Band Gaps with Hybrid Density Functionals. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4165-4170.	2.1	369
166	Polynomial similarity transformation theory: A smooth interpolation between coupled cluster doubles and projected BCS applied to the reduced BCS Hamiltonian. <i>Physical Review B</i> , 2016, 93, .	1.1	53
167	Ring-locking enables selective anhydrosugar synthesis from carbohydrate pyrolysis. <i>Green Chemistry</i> , 2016, 18, 5438-5447.	4.6	29
168	Communication: Projected Hartree Fock theory as a polynomial similarity transformation theory of single excitations. <i>Journal of Chemical Physics</i> , 2016, 145, .	1.2	28
169	The two pillars: density and spin-density functional theories. <i>Molecular Physics</i> , 2016, 114, 928-931.	0.8	6
170	Graphene Nanoribbons-Based Ultrasensitive Chemical Detectors. <i>Journal of Physical Chemistry C</i> , 2016, 120, 3791-3797.	1.5	11
171	Combinations of coupled cluster, density functionals, and the random phase approximation for describing static and dynamic correlation, and van der Waals interactions. <i>Molecular Physics</i> , 2016, 114, 997-1018.	0.8	23
172	Lie algebraic similarity transformed Hamiltonians for lattice model systems. <i>Physical Review B</i> , 2015, 91, .	1.1	23
173	Cluster-based mean-field and perturbative description of strongly correlated fermion systems: Application to the one- and two-dimensional Hubbard model. <i>Physical Review B</i> , 2015, 92, .	1.1	20
174	Actinide chemistry using singlet-paired coupled cluster and its combinations with density functionals. <i>Journal of Chemical Physics</i> , 2015, 143, 244106.	1.2	22
175	Seniority number description of potential energy surfaces: Symmetric dissociation of water, N ₂ , C ₂ , and Be ₂ . <i>Journal of Chemical Physics</i> , 2015, 143, 094105.	1.2	36
176	Solutions of the Two-Dimensional Hubbard Model: Benchmarks and Results from a Wide Range of Numerical Algorithms. <i>Physical Review X</i> , 2015, 5, .	2.8	398
177	Range separated hybrids of pair coupled cluster doubles and density functionals. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 22412-22422.	1.3	40
178	Can Single-Reference Coupled Cluster Theory Describe Static Correlation?. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3171-3179.	2.3	103
179	Synergy between pair coupled cluster doubles and pair density functional theory. <i>Journal of Chemical Physics</i> , 2015, 142, 044109.	1.2	36
180	On the equivalence of LIST and DIIS methods for convergence acceleration. <i>Journal of Chemical Physics</i> , 2015, 142, 164104.	1.2	7

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181	Pair extended coupled cluster doubles. <i>Journal of Chemical Physics</i> , 2015, 142, 214116.	1.2	53
182	Can Gap Tuning Schemes of Long-Range Corrected Hybrid Functionals Improve the Description of Hyperpolarizabilities?. <i>Journal of Physical Chemistry B</i> , 2015, 119, 1202-1212.	1.2	54
183	Seniority-based coupled cluster theory. <i>Journal of Chemical Physics</i> , 2014, 141, 244104.	1.2	110
184	Analytic energy gradient for the projected Hartree-Fock method. <i>Journal of Chemical Physics</i> , 2014, 140, 204101.	1.2	15
185	Symmetry-projected wave functions in quantum Monte Carlo calculations. <i>Physical Review B</i> , 2014, 89, .	1.1	43
186	Seniority zero pair coupled cluster doubles theory. <i>Journal of Chemical Physics</i> , 2014, 140, 214113.	1.2	147
187	Sign problem in full configuration interaction quantum Monte Carlo: Linear and sublinear representation regimes for the exact wave function. <i>Physical Review B</i> , 2014, 90, .	1.1	31
188	Variational description of the ground state of the repulsive two-dimensional Hubbard model in terms of nonorthogonal symmetry-projected Slater determinants. <i>Physical Review B</i> , 2014, 90, .	1.1	11
189	Range-Separated Brueckner Coupled Cluster Doubles Theory. <i>Physical Review Letters</i> , 2014, 112, 133002.	2.9	37
190	Can Short- and Middle-Range Hybrids Describe the Hyperpolarizabilities of Long-Range Charge-Transfer Compounds?. <i>Journal of Physical Chemistry A</i> , 2014, 118, 11787-11796.	1.1	52
191	Density matrix embedding from broken symmetry lattice mean fields. <i>Physical Review B</i> , 2014, 89, .	1.1	103
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361	Abinitiotheoretical study of arsine and trimethylgallium: The formation of GaAs by a stable adduct. <i>Journal of Chemical Physics</i> , 1992, 96, 3723-3731.	1.2	20
362	A comparison of the coupled cluster and internally contracted averaged coupled pair functional levels of theory for the calculation of the MCH ₂ ⁺ binding energies for M=Sc to Cu. <i>Journal of Chemical Physics</i> , 1992, 97, 7471-7473.	1.2	33
363	A coupled cluster study of the electron affinity of the oxygen atom. <i>Journal of Chemical Physics</i> , 1992, 96, 9025-9029.	1.2	19
364	A coupled cluster study of the equilibrium bond distance in methane. <i>Molecular Physics</i> , 1992, 75, 1099-1103.	0.8	3
365	Comparison of coupled cluster results with a hybrid of Hartree-Fock and density functional theory. <i>Journal of Chemical Physics</i> , 1992, 97, 7528-7530.	1.2	181
366	Analytic evaluation of energy gradients for the singles and doubles coupled cluster method including perturbative triple excitations: Theory and applications to FOOF and Cr ₂ . <i>Journal of Chemical Physics</i> , 1991, 94, 442-447.	1.2	253
367	Application of open-shell coupled cluster theory to the ground state of GaAs. <i>Theoretica Chimica Acta</i> , 1991, 80, 215-219.	0.9	8
368	A coupled cluster study of the classical barrier height of the F+H ₂ →FH+H reaction. <i>Journal of Chemical Physics</i> , 1991, 95, 7426-7436.	1.2	33
369	Abinitiotheoretical study of small GaAs clusters. <i>Journal of Chemical Physics</i> , 1991, 95, 6602-6606.	1.2	54
370	The infrared spectrum of cyclotetraoxygen, O ₄ : A theoretical investigation employing the single and double excitation coupled cluster method. <i>Journal of Chemical Physics</i> , 1990, 92, 6077-6080.	1.2	45
371	A coupled cluster study of As ₂ . <i>Journal of Chemical Physics</i> , 1990, 92, 6722-6727.	1.2	27
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374	Coupled cluster energy derivatives. Analytic Hessian for the closed shell coupled cluster singles and doubles wave function: Theory and applications. <i>Journal of Chemical Physics</i> , 1990, 92, 4924-4940.	1.2	222
375	The calculation of electric dipole moments from the polarization propagator. Theory and application. <i>Journal of Chemical Physics</i> , 1989, 91, 364-367.	1.2	10
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377	Is coupled cluster singles and doubles (CCSD) more computationally intensive than quadratic configuration interaction (QCISD)? <i>Journal of Chemical Physics</i> , 1989, 90, 3700-3703.	1.2	1,065
378	The electric dipole moment of ArH ⁺ . Disagreement between theory and experiment. <i>Journal of Chemical Physics</i> , 1989, 90, 6486-6490.	1.2	24

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379	Ordering of the O-O stretching vibrational frequencies in ozone. <i>Journal of Chemical Physics</i> , 1989, 90, 5635-5637.	1.2	40
380	A systematic theoretical study of harmonic vibrational frequencies: The single and double excitation coupled cluster (CCSD) method. <i>Journal of Chemical Physics</i> , 1988, 89, 360-366.	1.2	105
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382	Variational studies of the importance of triple and quadruple excitations on the barrier height for F+H ₂ →FH+H. <i>Journal of Chemical Physics</i> , 1988, 88, 7024-7026.	1.2	17
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384	Spin-spin coupling constants of CO and N ₂ . <i>Journal of Chemical Physics</i> , 1987, 87, 2138-2142.	1.2	82
385	The nuclear quadrupole moment of ¹⁴ N. A theoretical prediction from full valence shell and full configuration interaction atomic wave functions. <i>Journal of Chemical Physics</i> , 1987, 87, 4020-4024.	1.2	19
386	Analytic evaluation of energy gradients for the single and double excitation coupled cluster (CCSD) wave function: Theory and application. <i>Journal of Chemical Physics</i> , 1987, 87, 5361-5373.	1.2	378
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