

# Robert O Jones

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

173  
papers

12,323  
citations

52  
h-index

109  
g-index

186  
ext. papers

13,014  
ext. citations

4.6  
avg, IF

6.71  
L-index

#	Paper	IF	Citations
173	Phase change memory materials: Rationalizing the dominance of Ge/Sb/Te alloys. <i>Physical Review B</i> , <b>2020</b> , 101,	3.3	13
172	Density functional and classical simulations of liquid and glassy selenium. <i>Physical Review B</i> , <b>2020</b> , 102,	3.3	2
171	Bonding in phase change materials: concepts and misconceptions. <i>Journal of Physics Condensed Matter</i> , <b>2018</b> , 30, 153001	1.8	10
170	Speeding up crystallization. <i>Science</i> , <b>2017</b> , 358, 1386	33.3	12
169	Crystallization of supercooled liquid antimony: A density functional study. <i>Physical Review B</i> , <b>2017</b> , 96,	3.3	15
168	Density functional study of structure and dynamics in liquid antimony and Sb clusters. <i>Journal of Chemical Physics</i> , <b>2017</b> , 146, 194502	3.9	7
167	Tuning electronic properties of graphene heterostructures by amorphous-to-crystalline phase transitions. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	4
166	Crystallization processes in the phase change material Ge <sub>2</sub> Sb <sub>2</sub> Te <sub>5</sub> : Unbiased density functional/molecular dynamics simulations. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	40
165	Collective excitations and viscosity in liquid Bi. <i>Journal of Chemical Physics</i> , <b>2016</b> , 145, 184502	3.9	12
164	Structure of amorphous Ag/Ge/S alloys: experimentally constrained density functional study. <i>Journal of Physics Condensed Matter</i> , <b>2015</b> , 27, 485304	1.8	11
163	Density functional theory: Its origins, rise to prominence, and future. <i>Reviews of Modern Physics</i> , <b>2015</b> , 87, 897-923	40.5	666
162	The Prototype Phase Change Material ( $\text{Ge}_2\text{Sb}_2\text{Te}_5$ ): Amorphous Structure and Crystallization. <i>Springer Series in Materials Science</i> , <b>2015</b> , 457-484	0.9	
161	Simulation of crystallization in Ge <sub>2</sub> Sb <sub>2</sub> Te <sub>5</sub> : A memory effect in the canonical phase-change material. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	51
160	Structure, electronic, and vibrational properties of amorphous As <sub>2</sub> S <sub>3</sub> and AgAs <sub>2</sub> S <sub>3</sub> : Experimentally constrained density functional study. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	13
159	Structure and dynamics in liquid bismuth and Bi(n) clusters: a density functional study. <i>Journal of Chemical Physics</i> , <b>2014</b> , 141, 194503	3.9	17
158	Density functional simulations of structure and polymorphism in Ga/Sb films. <i>Journal of Physics Condensed Matter</i> , <b>2013</b> , 25, 115801	1.8	10
157	Amorphous structures of Ge/Sb/Te alloys: Density functional simulations. <i>Physica Status Solidi (B): Basic Research</i> , <b>2012</b> , 249, 1851-1860	1.3	24

156	Structure and dynamics in amorphous tellurium and Ten clusters: A density functional study. <i>Physical Review B</i> , <b>2012</b> , 85,	3-3	40
155	Nucleus-driven crystallization of amorphous Ge <sub>2</sub> Sb <sub>2</sub> Te <sub>5</sub> : A density functional study. <i>Physical Review B</i> , <b>2012</b> , 86,	3-3	66
154	Structure, electronic, and vibrational properties of glassy Ga <sub>11</sub> Ge <sub>11</sub> Te <sub>78</sub> : Experimentally constrained density functional study. <i>Physical Review B</i> , <b>2012</b> , 86,	3-3	36
153	Amorphous GeTe—density functional, high-energy x-ray and neutron diffraction study. <i>Journal of Physics Condensed Matter</i> , <b>2012</b> , 24, 015802	1.8	38
152	Density Functional Theory: A Personal View. <i>Springer Series in Solid-state Sciences</i> , <b>2012</b> , 1-28	0.4	5
151	From local structure to nanosecond recrystallization dynamics in AgInSbTe phase-change materials. <i>Nature Materials</i> , <b>2011</b> , 10, 129-34	27	204
150	Polymorphism in phase-change materials: melt-quenched and as-deposited amorphous structures in Ge <sub>2</sub> Sb <sub>2</sub> Te <sub>5</sub> from density functional calculations. <i>Physical Review B</i> , <b>2011</b> , 83,	3-3	64
149	Comment on "Formation of large voids in the amorphous phase-change memory Ge <sub>2</sub> Sb <sub>2</sub> Te <sub>5</sub> alloy". <i>Physical Review Letters</i> , <b>2010</b> , 104, 019603; author reply 019604	7-4	4
148	Density variations in liquid tellurium: Roles of rings, chains, and cavities. <i>Physical Review B</i> , <b>2010</b> , 81,	3-3	40
147	Structure of amorphous Ge <sub>8</sub> Sb <sub>2</sub> Te <sub>11</sub> : GeTe-Sb <sub>2</sub> Te <sub>3</sub> alloys and optical storage. <i>Physical Review B</i> , <b>2009</b> , 79,	3-3	53
146	Structure of liquid phase change material AgInSbTe from density functional/molecular dynamics simulations. <i>Applied Physics Letters</i> , <b>2009</b> , 94, 251905	3-4	21
145	Experimentally constrained density-functional calculations of the amorphous structure of the prototypical phase-change material Ge <sub>2</sub> Sb <sub>2</sub> Te <sub>5</sub> . <i>Physical Review B</i> , <b>2009</b> , 80,	3-3	73
144	Molecular calculations using the muffin-tin orbital method. <i>International Journal of Quantum Chemistry</i> , <b>2009</b> , 12, 71-74	2.1	
143	Density functional study of amorphous, liquid and crystalline Ge(2)Sb(2)Te(5): homopolar bonds and/or AB alternation?. <i>Journal of Physics Condensed Matter</i> , <b>2008</b> , 20, 465103	1.8	88
142	Binary alloys of Ge and Te: order, voids, and the eutectic composition. <i>Physical Review Letters</i> , <b>2008</b> , 100, 205502	7-4	103
141	Molecular Calculations with the Density Functional Formalism. <i>Advances in Chemical Physics</i> , <b>2007</b> , 413-437		10
140	Structural phase transitions on the nanoscale: The crucial pattern in the phase-change materials Ge <sub>2</sub> Sb <sub>2</sub> Te <sub>5</sub> and GeTe. <i>Physical Review B</i> , <b>2007</b> , 76,	3-3	373
139	Density functional calculations of ATP systems. 2. ATP hydrolysis at the active site of actin. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 8121-9	3-4	25

138	Density functional calculations of ATP systems. 1. Crystalline ATP hydrates and related molecules. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 8110-20	3.4	14
137	Ring-Opening and Branching in Polycarbonates: A Density Functional-Monte Carlo Study. <i>ACS Symposium Series</i> , <b>2005</b> , 200-213	0.4	
136	A reactive force field simulation of liquid-liquid phase transitions in phosphorus. <i>Journal of Chemical Physics</i> , <b>2004</b> , 121, 8147-57	3.9	26
135	Stability and structure of Li(n)H molecules (n=3-6): experimental and density functional study. <i>Journal of Chemical Physics</i> , <b>2004</b> , 120, 5128-32	3.9	14
134	Smallest carbon nanotube is 3 a in diameter. <i>Physical Review Letters</i> , <b>2004</b> , 92, 125502	7.4	244
133	ATP Hydrolysis in Water [A Density Functional Study. <i>Journal of Physical Chemistry B</i> , <b>2003</b> , 107, 11774-11783	3.5	86
132	Branching Reactions in Polycarbonate: A Density Functional Study. <i>Macromolecules</i> , <b>2003</b> , 36, 1355-1360	3.5	10
131	Density functional and Monte Carlo studies of sulfur. I. Structure and bonding in Sn rings and chains (n=2-8). <i>Journal of Chemical Physics</i> , <b>2003</b> , 118, 9257-9265	3.9	57
130	Carbon species confined inside carbon nanotubes: A density functional study. <i>Physical Review B</i> , <b>2003</b> , 68,	3.3	73
129	Density functional and Monte Carlo studies of sulfur. II. Equilibrium polymerization of the liquid phase. <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 8704-8715	3.9	16
128	Density functional/Monte Carlo study of ring-opening polymerization. <i>Computer Physics Communications</i> , <b>2002</b> , 147, 325-330	4.2	2
127	Equilibrium polymerization of cyclic carbonate oligomers. III. Chain branching and the gel transition. <i>Journal of Chemical Physics</i> , <b>2002</b> , 117, 6841-6851	3.9	9
126	Equilibrium polymerization of cyclic carbonate oligomers. II. Role of multiple active sites. <i>Journal of Chemical Physics</i> , <b>2002</b> , 116, 7724-7732	3.9	6
125	Reactions of Polycarbonate with Cyclohexene Oxide and Phosphites: [A Density Functional Study. <i>Macromolecules</i> , <b>2002</b> , 35, 2327-2334	5.5	4
124	Si-H clusters, defects, and hydrogenated silicon. <i>Physical Review B</i> , <b>2001</b> , 64,	3.3	16
123	Density functional calculations for polymers and clusters [progress and limitations. <i>Computational Materials Science</i> , <b>2001</b> , 22, 1-6	3.2	3
122	Equilibrium polymerization of cyclic carbonate oligomers. <i>Journal of Chemical Physics</i> , <b>2001</b> , 115, 3895-3905	3.9	12
121	Density Functional Study of Reactions of Phenoxides with Polycarbonate. <i>Journal of Physical Chemistry A</i> , <b>2001</b> , 105, 3008-3015	2.8	14

120	A Combined Density Functional and Monte Carlo Study of Polycarbonate. <i>Materials Research Society Symposia Proceedings</i> , <b>2001</b> , 677, 311		
119	Anisotropic thermal expansion in silicates: A density functional study of Eucryptite and related materials. <i>Physical Review B</i> , <b>2000</b> , 62, 11487-11493	3.3	43
118	Density functional study of carbonic acid clusters. <i>Journal of Chemical Physics</i> , <b>2000</b> , 112, 6571-6575	3.9	27
117	Catalytic Reactions of Living Polymers: Density Functional Study of Reactivity of Phenol and Phenoxides with the Cyclic Tetramer of Polycarbonate. <i>Journal of Physical Chemistry A</i> , <b>2000</b> , 104, 2793-2798	2.8	17
116	Density functional theory and molecular bonding. I. First-row diatomic molecules. <i>Journal of Chemical Physics</i> , <b>1999</b> , 67, 3970	3.9	135
115	Cluster geometries from density functional calculations [prospects and limitations]. <i>European Physical Journal D</i> , <b>1999</b> , 9, 81-84	1.3	2
114	Density functional study of carbon clusters C <sub>2n</sub> (2 ≤ n ≤ 16). I. Structure and bonding in the neutral clusters. <i>Journal of Chemical Physics</i> , <b>1999</b> , 110, 5189-5200	3.9	158
113	Density Functional Study of Polycarbonate. 2. Crystalline Analogs, Cyclic Oligomers, and Their Fragments. <i>Macromolecules</i> , <b>1999</b> , 32, 3396-3404	5.5	22
112	Polycarbonate Simulations with a Density Functional Based Force Field. <i>Journal of Physical Chemistry A</i> , <b>1999</b> , 103, 5387-5398	2.8	15
111	Cluster geometries from density functional calculations [prospects and limitations] <b>1999</b> , 81-84		
110	Density Functional Study of Crystalline Analogs of Polycarbonates. <i>Macromolecules</i> , <b>1998</b> , 31, 7784-7790	5.5	14
109	Density functional study of molecular crystals: Polyethylene and a crystalline analog of bisphenol-A polycarbonate. <i>Journal of Chemical Physics</i> , <b>1998</b> , 108, 6947-6951	3.9	38
108	Anisotropic thermal expansion in the silicate Eucryptite: A neutron diffraction and density functional study. <i>Physical Review B</i> , <b>1998</b> , 58, 6219-6223	3.3	38
107	Density Functional Calculations for Molecules and Clusters [Lin, LinO, C <sub>n</sub> ] <b>1998</b> , 349-360		1
106	Density functional study of polypropylene and its submolecules. <i>Journal of Chemical Physics</i> , <b>1997</b> , 106, 8545-8551	3.9	18
105	Density functional study of structure and bonding in lithium clusters Lin and their oxides LinO. <i>Journal of Chemical Physics</i> , <b>1997</b> , 106, 4566-4574	3.9	106
104	Structure and Bonding in Carbon Clusters C <sub>14</sub> to C <sub>24</sub> : Chains, Rings, Bowls, Plates, and Cages. <i>Physical Review Letters</i> , <b>1997</b> , 79, 443-446	7.4	163
103	Density functional study of crystalline polyethylene. <i>Chemical Physics Letters</i> , <b>1997</b> , 272, 347-352	2.5	45

102	Structure and bonding in mixed silicon-carbon clusters and their anions. <i>Journal of Chemical Physics</i> , <b>1996</b> , 105, 5048-5060	3.9	81
101	Model interatomic potential for simulations in selenium. <i>Physical Review B</i> , <b>1996</b> , 53, 6165-6173	3.3	65
100	Structure and spectroscopy of small atomic clusters. <i>Topics in Current Chemistry</i> , <b>1996</b> , 87-118		1
99	Rings and chains in sulfur cluster anions S <sub>n</sub> <sup>-</sup> to S <sub>9</sub> <sup>-</sup> . Theory (simulated annealing) and experiment (photoelectron detachment). <i>Journal of Chemical Physics</i> , <b>1995</b> , 102, 5917-5936	3.9	78
98	Structure and spectroscopy of phosphorus cluster anions: Theory (simulated annealing) and experiment (photoelectron detachment). <i>Journal of Chemical Physics</i> , <b>1995</b> , 103, 9549-9562	3.9	74
97	Structure and spin in small iron clusters. <i>Chemical Physics Letters</i> , <b>1995</b> , 233, 632-638	2.5	119
96	Prediction and observation of ring and chain isomers in Sn <sub>n</sub> <sup>-</sup> ions. <i>Chemical Physics Letters</i> , <b>1995</b> , 236, 43-49	2.5	20
95	Density Functionals, Molecular Dynamics, and More <b>1995</b> , 37-66		
94	Molecules and Molecular Dynamics. <i>NATO ASI Series Series B: Physics</i> , <b>1995</b> , 273-297		
93	Polymerization in liquid phosphorus: Simulation of a phase transition. <i>Physical Review B</i> , <b>1994</b> , 50, 17047-17053	3.1	149
92	Density functional study of phosphorus and arsenic clusters using local and nonlocal energy functionals. <i>Journal of Chemical Physics</i> , <b>1994</b> , 100, 4941-4946	3.9	96
91	Isomers of S <sub>7</sub> O <sub>2</sub> : A Simulated Annealing Study. <i>Inorganic Chemistry</i> , <b>1994</b> , 33, 1340-1343	5.1	2
90	Theoretical Concepts. <i>Springer Series in Chemical Physics</i> , <b>1994</b> , 13-205	0.3	2
89	Simulated annealing study of neutral and charged clusters: Al <sub>n</sub> and Ga <sub>n</sub> . <i>Journal of Chemical Physics</i> , <b>1993</b> , 99, 1194-1206	3.9	175
88	Aluminum and gallium clusters: A comparative study using simulated annealing. <i>Zeitschrift für Physik D-Atoms Molecules and Clusters</i> , <b>1993</b> , 26, 23-27		8
87	Structure of phosphorus clusters by simulated annealing. <i>Zeitschrift für Physik D-Atoms Molecules and Clusters</i> , <b>1993</b> , 26, 349-351		9
86	Structural Trends in Clusters and Disordered Systems. <i>Springer Series in Solid-state Sciences</i> , <b>1993</b> , 67-76	0.4	
85	Cage molecules containing elements of groups V and VI. II. Molecular dynamics study of P <sub>4</sub> S <sub>3</sub> and P <sub>3</sub> S <sub>4</sub> . <i>Journal of Chemical Physics</i> , <b>1992</b> , 96, 2951-2952	3.9	21

84	Amorphous phosphorus: A cluster-network model. <i>Physical Review B</i> , <b>1992</b> , 45, 8995-9005	3.3	27
83	Cage molecules containing elements of groups V and VI. I. Structure determinations using simulated annealing. <i>Journal of Chemical Physics</i> , <b>1992</b> , 96, 2942-2950	3.9	20
82	Structure of phosphorus clusters using simulated annealing. II. P <sub>9</sub> , P <sub>10</sub> , P <sub>11</sub> , anions P <sub>2</sub> <sup>-</sup> , P <sub>2</sub> <sup>0</sup> , P <sub>3</sub> <sup>-</sup> , and cations P <sub>n</sub> <sup>+</sup> to n=11. <i>Journal of Chemical Physics</i> , <b>1992</b> , 96, 7564-7572	3.9	91
81	Structure and bonding in aluminium and gallium clusters <b>1992</b> , 305-311		
80	Molecular Structures from Density Functional Calculations with Simulated Annealing. <i>Angewandte Chemie International Edition in English</i> , <b>1991</b> , 30, 630-640		19
79	Die Berechnung von Molekülstrukturen durch eine Kombination von Dichtefunktional- und Moleküldynamikmethoden. <i>Angewandte Chemie</i> , <b>1991</b> , 103, 647-657	3.6	7
78	Geometric and electronic structure of clusters. <i>Zeitschrift für Physik D-Atoms Molecules and Clusters</i> , <b>1991</b> , 20, 77-80		38
77	First-principles molecular-dynamics simulation of liquid and amorphous selenium. <i>Physical Review B</i> , <b>1991</b> , 43, 3856-3870	3.3	151
76	Density Functional Calculations - A Database for Parameterizing Interatomic Potentials <b>1991</b> , 437-450		
75	Structure and bonding in small aluminum clusters. <i>Physical Review Letters</i> , <b>1991</b> , 67, 224-227	7.4	117
74	Density functional calculations with simulated annealing clusters and amorphous materials. <i>Physica Scripta</i> , <b>1991</b> , T35, 154-158	2.6	4
73	Geometric and electronic structure of clusters <b>1991</b> , 527-530		
72	Density functional calculations with simulated annealing isomers of S <sub>7</sub> X [X = O, S, Se], Se <sub>8</sub> , O <sub>8</sub> . <i>International Journal of Quantum Chemistry</i> , <b>1990</b> , 38, 141-151	2.1	12
71	Structure, bonding, and dynamics in heterocyclic sulfur-selenium molecules, SexSy. <i>Journal of the American Chemical Society</i> , <b>1990</b> , 112, 2590-2596	16.4	36
70	First principles MD simulation of liquid and amorphous selenium. <i>Journal of Non-Crystalline Solids</i> , <b>1990</b> , 117-118, 922-925	3.9	19
69	Structure of phosphorus clusters using simulated annealing P <sub>2</sub> to P <sub>8</sub> . <i>Journal of Chemical Physics</i> , <b>1990</b> , 92, 6710-6721	3.9	168
68	Simulated Annealing Studies of Sulphur and Selenium Clusters. <i>Springer Proceedings in Physics</i> , <b>1990</b> , 214-231	0.2	1
67	Density Functional Calculations with Simulated Annealing [New Perspectives for Molecular Calculations <b>1990</b> , 127-142		

66	Energy surfaces and structure of <i>STO</i> . <i>Journal of the American Chemical Society</i> , <b>1989</b> , 111, 825-828	16.4	27
65	The density functional formalism, its applications and prospects. <i>Reviews of Modern Physics</i> , <b>1989</b> , 61, 689-746	40.5	3143
64	LEED fine structure: Origins and applications. <i>Surface Science Reports</i> , <b>1988</b> , 9, 165-196	12.9	74
63	Sulfur and selenium helices: Structure and electronic properties. <i>Journal of Chemical Physics</i> , <b>1988</b> , 88, 2652-2658	3.9	65
62	Structure of sulfur clusters using simulated annealing: S <sub>2</sub> to S <sub>13</sub> . <i>Journal of Chemical Physics</i> , <b>1988</b> , 89, 6823-6835	3.9	198
61	Beyond the method of images—the interaction of charged particles with real surfaces. <i>Advances in Physics</i> , <b>1988</b> , 37, 341-358	18.4	58
60	Surface barrier for electrons in metals. <i>Physical Review B</i> , <b>1988</b> , 37, 6113-6120	3.3	240
59	The structure of selenium clusters [Se <sub>3</sub> TO Se <sub>8</sub> ]. <i>Chemical Physics Letters</i> , <b>1987</b> , 139, 540-545	2.5	156
58	Density-functional formalism: <i>V<sub>xc</sub></i> , discontinuities, and the local density approximation. <i>Lecture Notes in Physics</i> , <b>1987</b> , 77-92	0.8	
57	Electronic structure of <i>so<sub>s</sub></i> - a comparison with O <sub>3</sub> , SO <sub>2</sub> , and S <sub>3</sub> . <i>Chemical Physics Letters</i> , <b>1986</b> , 125, 221-224	2.4	15
56	Surface barrier in W(110). I. Self-consistent film calculations. <i>Physical Review B</i> , <b>1986</b> , 34, 6695-6698	3.3	15
55	Low-lying states of thiozone, S <sub>3</sub> . <i>Journal of Chemical Physics</i> , <b>1986</b> , 84, 318-322	3.9	31
54	Surface barrier in W(110). II. Low-energy electron diffraction fine-structure analysis. <i>Physical Review B</i> , <b>1986</b> , 34, 6699-6703	3.3	13
53	Energy surfaces of polymeric sulfur: Structure and electronic properties. <i>Physical Review Letters</i> , <b>1986</b> , 57, 1145-1148	7.4	30
52	Chemisorption and surface barrier structure. <i>Surface Science</i> , <b>1986</b> , 176, 691-700	1.8	11
51	Reply to Comment: On the equilibrium of Hg <sub>2</sub> molecule— <i>Journal of Chemical Physics</i> , <b>1985</b> , 83, 2622-2623	0.9	
50	Surface barrier studies with LEED fine structure analysis. <i>Applications of Surface Science</i> , <b>1985</b> , 22-23, 35-47		
49	Energy surfaces for Si <sub>3</sub> and C <sub>3</sub> : A comparative study. <i>Physical Review A</i> , <b>1985</b> , 32, 2589-2594	2.6	32



48	Low-energy-electron-diffraction fine structure in W(001) for energies from 0 to 35 eV. <i>Physical Review B</i> , <b>1985</b> , 32, 6131-6137	3.3	27
47	Total-energy differences: Sources of error in local-density approximations. <i>Physical Review B</i> , <b>1985</b> , 31, 7588-7602	3.3	161
46	Density-functional formalism: Sources of error in local-density approximations. <i>Physical Review Letters</i> , <b>1985</b> , 55, 107-110	7.4	33
45	Energy surfaces of low-lying states of C3. <i>Journal of Chemical Physics</i> , <b>1985</b> , 82, 5078-5083	3.9	17
44	Energy surfaces of low-lying states of O3 and SO2. <i>Journal of Chemical Physics</i> , <b>1985</b> , 82, 325-332	3.9	84
43	Density-Functional Calculations for Ozone: Striking Results for an Important Molecule. <i>Physical Review Letters</i> , <b>1984</b> , 52, 2002-2005	7.4	16
42	Surface barrier in metals: A new model with application to W(001). <i>Physical Review B</i> , <b>1984</b> , 29, 6474-6483	3.3	172
41	Schwerpunkt '84: Physikalische Forschung mit dem Computer: Das Dichtefunktional Die Methode zur Berechnung von Bindungseigenschaften?. <i>Physik Journal</i> , <b>1984</b> , 40, 149-152		3
40	Exchange-Correlation Energy Functionals in the Density Functional Formalism <b>1984</b> , 229-243		1
39	Fine-structure analysis of spin-polarized low-energy electron diffraction from W(001). <i>Physical Review B</i> , <b>1983</b> , 27, 4702-4711	3.3	29
38	Density functional calculations for H2O, NH3, and CO2 using localized muffin-tin orbitals. <i>Journal of Chemical Physics</i> , <b>1983</b> , 79, 1874-1884	3.9	50
37	Density functional calculations for low-lying states of CO2. <i>Journal of Chemical Physics</i> , <b>1983</b> , 79, 1885-1890	3.9	13
36	Energy differences using an accurate local density functional. <i>Journal of Chemical Physics</i> , <b>1982</b> , 76, 3098-3101	3.3	36
35	Surface barrier determination using spin-polarized LEED: W(001). <i>Solid State Communications</i> , <b>1982</b> , 44, 17-22	1.6	14
34	Self-interaction corrections in the density functional formalism. <i>Solid State Communications</i> , <b>1981</b> , 37, 249-252	1.6	50
33	Force calculations in the density functional formalism. <i>Journal of Chemical Physics</i> , <b>1981</b> , 75, 3904-3908	3.9	57
32	Density Functional Calculations for Atoms, Molecules and Clusters. <i>Physica Scripta</i> , <b>1980</b> , 21, 394-401	2.6	216
31	Molecular bonding in LiBe, LiMg, and LiCa. <i>Journal of Chemical Physics</i> , <b>1980</b> , 72, 3197-3200	3.9	33

30	Extensions of the LSD approximation in density functional calculations. <i>Journal of Chemical Physics</i> , <b>1980</b> , 72, 5357-5362	3.9	71
29	Bonding trends in the group-IVA dimers C <sub>2</sub> -Pb <sub>2</sub> . <i>Physical Review A</i> , <b>1979</b> , 19, 1813-1818	2.6	39
28	Molecular bonding in Group IIA dimers Be <sub>2</sub> Ba <sub>2</sub> . <i>Journal of Chemical Physics</i> , <b>1979</b> , 71, 1300-1308	3.9	150
27	Density functional theory and molecular bonding. III. Iron-series dimers. <i>Journal of Chemical Physics</i> , <b>1979</b> , 70, 830	3.9	233
26	Density Functional Calculations for Atomic Clusters <b>1979</b> , 55-70		
25	Spin-dependent features in leed intensity curves. <i>Surface Science</i> , <b>1978</b> , 71, 101-106	1.8	19
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