Robert O Jones

List of Publications by Year
in descending order

176	13,752	31902	21474
papers	citations	53 h-index	114 g-index

186	186	186	8129
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The density functional formalism, its applications and prospects. Reviews of Modern Physics, 1989, 61, 689-746.	16.4	3,538
2	Density functional theory: Its origins, rise to prominence, and future. Reviews of Modern Physics, 2015, 87, 897-923.	16.4	962
3	The surface energy of a bounded electron gas. Journal of Physics F: Metal Physics, 1974, 4, 1170-1186.	1.6	433
4	Structural phase transitions on the nanoscale: The crucial pattern in the phase-change materials<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Ge</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">Sb</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">Te</mml:mi><mml:mn>5</mml:mn></mml:msub></mml:mrow></mml:math>and G	1.1	417
5	Smallest Carbon Nanotube Is3â€‰â€‰Ã…in Diameter. Physical Review Letters, 2004, 92, 125502.	2.9	272
6	Surface barrier for electrons in metals. Physical Review B, 1988, 37, 6113-6120.	1.1	256
7	Density functional theory and molecular bonding. III. Iron-series dimers. Journal of Chemical Physics, 1979, 70, 830.	1.2	240
8	From local structure to nanosecond recrystallization dynamics in AgInSbTeÂphase-changeÂmaterials. Nature Materials, 2011, 10, 129-134.	13.3	238
9	Density Functional Calculations for Atoms, Molecules and Clusters. Physica Scripta, 1980, 21, 394-401.	1.2	224
10	Structure of sulfur clusters using simulated annealing: S2to S13. Journal of Chemical Physics, 1988, 89, 6823-6835.	1.2	214
11	Electronic band structure and covalency in diamond-type semiconductors. Journal of Physics C: Solid State Physics, 1969, 2, 719-732.	1.5	203
12	Simulated annealing study of neutral and charged clusters: Alnand Gan. Journal of Chemical Physics, 1993, 99, 1194-1206.	1.2	193
13	Structure of phosphorus clusters using simulated annealingâ€”P2 to P8. Journal of Chemical Physics, 1990, 92, 6710-6721.	1.2	188
14	Surface barrier in metals: A new model with application to W(001). Physical Review B, 1984, 29, 6474-6480.	1.1	178
15	Density functional study of carbon clusters C2n (2â©½nâ©½16). I. Structure and bonding in the neutral clusters. Journal of Chemical Physics, 1999, 110, 5189-5200.	1.2	174
16	Total-energy differences: Sources of error in local-density approximations. Physical Review B, 1985, 31, 7588-7602.	1.1	169
17	Structure and Bonding in Carbon ClustersC14toC24: Chains, Rings, Bowls, Plates, and Cages. Physical Review Letters, 1997, 79, 443-446.	2.9	167
18	The structure of selenium clusters â€” Se3 TO Se8. Chemical Physics Letters, 1987, 139, 540-545.	1.2	166

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19	First-principles molecular-dynamics simulation of liquid and amorphous selenium. Physical Review B, 1991, 43, 3856-3870.	1.1	162
20	Molecular bonding in Group IIA dimers Be2â€“Ba2. Journal of Chemical Physics, 1979, 71, 1300-1308.	1.2	159
21	Density functional theory and molecular bonding. I. First-row diatomic molecules. Journal of Chemical Physics, 1999, 67, 3970.	1.2	139
22	Muffin-tin orbitals and the total energy of atomic clusters. Physical Review B, 1977, 15, 3027-3038.	1.1	136
23	Structure and bonding in small aluminum clusters. Physical Review Letters, 1991, 67, 224-227.	2.9	124
24	Structure and spin in small iron clusters. Chemical Physics Letters, 1995, 233, 632-638.	1.2	122
25	Density functional study of structure and bonding in lithium clusters Lin and their oxides LinO. Journal of Chemical Physics, 1997, 106, 4566-4574.	1.2	117
26	Binary Alloys of Ge and Te: Order, Voids, and the Eutectic Composition. Physical Review Letters, 2008, 100, 205502.	2.9	110
27	Density functional study of phosphorus and arsenic clusters using local and nonlocal energy functionals. Journal of Chemical Physics, 1994, 100, 4941-4946.	1.2	103
28	Structure of phosphorus clusters using simulated annealing. II. P9, P10, P11, anions P2â^'4, P2â^'10, P3â^'11, and cations P+n to n=11. Journal of Chemical Physics, 1992, 96, 7564-7572.	1.2	102
29	Density functional study of amorphous, liquid and crystalline Ge₂Sb₂Te₅: homopolar bonds and/or AB alternation?. Journal of Physics Condensed Matter, 2008, 20, 465103.	0.7	102
30	ATP Hydrolysis in Water â^' A Density Functional Study. Journal of Physical Chemistry B, 2003, 107, 11774-11783.	1.2	97
31	Energy surfaces of lowâ€lying states of O3 and SO2. Journal of Chemical Physics, 1985, 82, 325-332.	1.2	87
32	Rings and chains in sulfur cluster anions Sâ^'to S9â^': Theory (simulated annealing) and experiment (photoelectron detachment). Journal of Chemical Physics, 1995, 102, 5917-5936.	1.2	85
33	Structure and bonding in mixed siliconâ€“carbon clusters and their anions. Journal of Chemical Physics, 1996, 105, 5048-5060.	1.2	83
34	Structure and spectroscopy of phosphorus cluster anions: Theory (simulated annealing) and experiment (photoelectron detachment). Journal of Chemical Physics, 1995, 103, 9549-9562.	1.2	81
35	Model interatomic potential for simulations in selenium. Physical Review B, 1996, 53, 6165-6173.	1.1	79
36	Carbon species confined inside carbon nanotubes:â€ƒA density functional study. Physical Review B, 2003, 68, .	1.1	79

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37	Pressure driven crystallization of amorphous Ge<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Sb<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Te<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mml:	1.1	79
38	LEED fine structure: Origins and applications. Surface Science Reports, 1988, 9, 165-196.	3.8	78
39	Experimentally constrained density-functional calculations of the amorphous structure of the prototypical phase-change materialGe2Sb2Te5. Physical Review B, 2009, 80, .	1.1	77
40	Dynamical corrections to the image potential. Journal of Physics C: Solid State Physics, 1973, 6, 3585-3604.	1.5	76
41	Polymorphism in phase-change materials: melt-quenched and as-deposited amorphous structures in Ge<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>Sb<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow	1.1	75
42	Extensions of the LSD approximation in density functional calculations. Journal of Chemical Physics, 1980, 72, 5357-5362.	1.2	74
43	Intrinsic Surface States in Semiconductors. Physical Review Letters, 1968, 20, 992-994.	2.9	72
44	Density functional theory of 3dâ€transition element atoms. Journal of Chemical Physics, 1978, 68, 3316-3317.	1.2	72
45	Density functional theory and molecular bonding. II. Alkali dimers. Journal of Chemical Physics, 1978, 68, 1190-1193.	1.2	70
46	Sulfur and selenium helices: Structure and electronic properties. Journal of Chemical Physics, 1988, 88, 2652-2658.	1.2	69
47	Low-Energy Electron-Diffraction Intensity Calculations for Beryllium with a Realistic Crystal Potential. Physical Review B, 1971, 3, 3228-3243.	1.1	68
48	Density functional and Monte Carlo studies of sulfur. I. Structure and bonding in Sn rings and chains (n=2â€“18). Journal of Chemical Physics, 2003, 118, 9257-9265.	1.2	68
49	Simulation of crystallization in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Ge</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">Sb</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">Te</mml:mi><mml:mn>5</mml:mn></mml:msub></mml:math>: A memory effect in the canonical phase-change material. Physical Review B, 2014, 90,	1.1	68
50	Beyond the method of imagesâ€”the interaction of charged particles with real surfaces. Advances in Physics, 1988, 37, 341-358.	35.9	62
51	Force calculations in the density functional formalism. Journal of Chemical Physics, 1981, 75, 3904-3908.	1.2	59
52	Structure of amorphousGe8Sb2Te11:GeTe-Sb2Te3alloys and optical storage. Physical Review B, 2009, 79, .	1.1	58
53	Image force for a moving charge. Journal of Physics C: Solid State Physics, 1974, 7, 3751-3754.	1.5	57
54	Crystallization processes in the phase change material <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="bold">Ge</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">Sb</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">Te</mml:mi><mml:mn>5</mml:mn></mml:msub></mml:mrow></mml:math> : Unbiased density functional/molecular dynamics simulations. Physical Review B, 2016, 94, .	1.1	57

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55	Anisotropic thermal expansion in silicates: A density functional study ofÎ²-eucryptite and related materials. Physical Review B, 2000, 62, 11487-11493.	1.1	53
56	Density functional calculations for H2O, NH3, and CO2 using localized muffinâ€tin orbitals. Journal of Chemical Physics, 1983, 79, 1874-1884.	1.2	52
57	Self-interaction corrections in the density functional formalism. Solid State Communications, 1981, 37, 249-252.	0.9	51
58	Polymerization in liquid phosphorus: Simulation of a phase transition. Physical Review B, 1994, 50, 17047-17053.	1.1	51
59	Structure and dynamics in amorphous tellurium and Te<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>n</mml:mi></mml:msub></mml:math>clusters: A density functional study. Physical Review B, 2012, 85, .	1.1	51
60	Inelastic Effects in Low-Energy Electron Diffraction. Physical Review Letters, 1969, 22, 1186-1188.	2.9	49
61	Anisotropic thermal expansion in the silicateÎ²-eucryptite: A neutron diffraction and density functional study. Physical Review B, 1998, 58, 6219-6223.	1.1	49
62	Pseudopotentials in Density-Functional Theory. Physical Review Letters, 1978, 41, 191-194.	2.9	48
63	Density variations in liquid tellurium: Roles of rings, chains, and cavities. Physical Review B, 2010, 81, .	1.1	48
64	Density functional study of crystalline polyethylene. Chemical Physics Letters, 1997, 272, 347-352.	1.2	47
65	Low-Energy Electron-Diffraction Intensity Calculations with a Realistic Crystal Potential. Physical Review Letters, 1970, 25, 516-520.	2.9	46
66	Multiplet structure and charge distributions in silicon and germanium dimers. Physical Review A, 1978, 18, 2159-2166.	1.0	45
67	Surface representations and complex band structure of a diamond-type semiconductor. Proceedings of the Physical Society, 1966, 89, 443-451.	1.6	44
68	Amorphous Ge₁₅Te₈₅: density functional, high-energy x-ray and neutron diffraction study. Journal of Physics Condensed Matter, 2012, 24, 015802.	0.7	43
69	Bonding trends in the group-IVAdimersC2-Pb2. Physical Review A, 1979, 19, 1813-1818.	1.0	42
70	pyMolDyn: Identification, structure, and properties of cavities/vacancies in condensed matter and molecules. Journal of Computational Chemistry, 2017, 38, 389-394.	1.5	42
71	Density functional study of molecular crystals: Polyethylene and a crystalline analog of bisphenol-A polycarbonate. Journal of Chemical Physics, 1998, 108, 6947-6951.	1.2	41
72	Structure, electronic, and vibrational properties of glassy Ga<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>11</mml:mn></mml:msub></mml:math>Ge<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>11</mml:mn></mml:msub></mml:math>Te<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mml:	1.1	41

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73	Structure, bonding, and dynamics in heterocyclic sulfur-selenium molecules, SexSy. Journal of the American Chemical Society, 1990, 112, 2590-2596.	6.6	40
74	Geometric and electronic structure of clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1991, 20, 77-80.	1.0	40
75	Cluster calculations of the electronic structure of transition metal surfaces. Surface Science, 1975, 53, 409-428.	0.8	37
76	Energy differences using an accurate local density functional. Journal of Chemical Physics, 1982, 76, 3098-3101.	1.2	37
77	Density-functional formalism: Sources of error in local-density approximations. Physical Review Letters, 1985, 55, 107-110.	2.9	37
78	Molecular bonding in LiBe, LiMg, and LiCa. Journal of Chemical Physics, 1980, 72, 3197-3200.	1.2	36
79	Energy Surfaces of Polymeric Sulfur: Structure and Electronic Properties. Physical Review Letters, 1986, 57, 1145-1148.	2.9	34
80	Energy surfaces forSi3andC3: A comparative study. Physical Review A, 1985, 32, 2589-2594.	1.0	32
81	Lowâ€lying states of thiozone, S3. Journal of Chemical Physics, 1986, 84, 318-322.	1.2	32
82	Fine-structure analysis of spin-polarized low-energy electron diffraction from W(001). Physical Review B, 1983, 27, 4702-4711.	1.1	31
83	Energy surfaces and structure of S7O. Journal of the American Chemical Society, 1989, 111, 825-828.	6.6	31
84	A reactive force field simulation of liquidâ€“liquid phase transitions in phosphorus. Journal of Chemical Physics, 2004, 121, 8147.	1.2	31
85	Low-energy-electron-diffraction fine structure in W(001) for energies from 0 to 35 eV. Physical Review B, 1985, 32, 6131-6137.	1.1	30
86	Model calculation of surface states in silicon. Journal of Physics C: Solid State Physics, 1972, 5, 1615-1628.	1.5	29
87	Amorphous phosphorus: A cluster-network model. Physical Review B, 1992, 45, 8995-9005.	1.1	28
88	Density Functional Calculations of ATP Systems. 2. ATP Hydrolysis at the Active Site of Actin. Journal of Physical Chemistry B, 2006, 110, 8121-8129.	1.2	28
89	Density functional study of carbonic acid clusters. Journal of Chemical Physics, 2000, 112, 6571-6575.	1.2	27
90	Density functional and Monte Carlo studies of sulfur. II. Equilibrium polymerization of the liquid phase. Journal of Chemical Physics, 2003, 119, 8704-8715.	1.2	25

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91	Amorphous structures of Ge/Sb/Te alloys: Density functional simulations. Physica Status Solidi (B): Basic Research, 2012, 249, 1851-1860.	0.7	25
92	Spin-polarization in LEED: A comparison of theoretical predictions. Surface Science, 1976, 61, 307-316.	0.8	23
93	Cage molecules containing elements of groups V and VI. I. Structure determinations using simulated annealing. Journal of Chemical Physics, 1992, 96, 2942-2950.	1.2	23
94	Density Functional Study of Polycarbonate. 2. Crystalline Analogs, Cyclic Oligomers, and Their Fragments. Macromolecules, 1999, 32, 3396-3404.	2.2	23
95	Structure of liquid phase change material AgInSbTe from density functional/molecular dynamics simulations. Applied Physics Letters, 2009, 94, 251905.	1.5	23
96	Electronic structure of stepped transition metal surfaces. Journal of Physics C: Solid State Physics, 1975, 8, L199-L202.	1.5	22
97	Cage molecules containing elements of groups V and VI. II. Molecular dynamics study of P4S3and P3â^'7. Journal of Chemical Physics, 1992, 96, 2951-2952.	1.2	22
98	Prediction and observation of ring and chain isomers in Snâ^' i ons. Chemical Physics Letters, 1995, 236, 43-49.	1.2	22
99	Phase change memory materials: Rationalizing the dominance of Ge/Sb/Te alloys. Physical Review B, 2020, 101, .	1.1	22
100	Molecular Structures from Density Functional Calculations with Simulated Annealing. Angewandte Chemie International Edition in English, 1991, 30, 630-640.	4.4	21
101	Structure and dynamics in liquid bismuth and Bin clusters: A density functional study. Journal of Chemical Physics, 2014, 141, 194503.	1.2	21
102	Spin-dependent features in leed intensity curves. Surface Science, 1978, 71, 101-106.	0.8	20
103	First principles MD simulation of liquid and amorphous selenium. Journal of Non-Crystalline Solids, 1990, 117-118, 922-925.	1.5	20
104	Crystallization of supercooled liquid antimony: A density functional study. Physical Review B, 2017, 96, .	1.1	20
105	Intensities of Low-Energy-Electron-Diffraction Beams from Be(0001). Physical Review B, 1972, 6, 407-416.	1.1	19
106	Density functional study of polypropylene and its submolecules. Journal of Chemical Physics, 1997, 106, 8545-8551.	1.2	19
107	Catalytic Reactions of Living Polymers:Â Density Functional Study of Reactivity of Phenol and Phenoxides with the Cyclic Tetramer of Polycarbonate. Journal of Physical Chemistry A, 2000, 104, 2793-2798.	1.1	18
108	Structure, electronic, and vibrational properties of amorphous<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>AsS</mml:mtext><mml:mn>2</mml:mn></mml:msub xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mtext>Ag</mml:mtext><mml:msub><mml:mtext>AsS</mml:mtext><mml:mtext><mml Experimentally constrained density functional study. Physical Review B, 2014, 89, .	1.1	18

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109	On the existence of Stark ladders in finite crystals. Journal of Physics C: Solid State Physics, 1972, 5, 2149-2155.	1.5	17
110	Local densities of states and bonding properties of 3d-transition metal clusters. Surface Science, 1976, 61, 255-271.	0.8	17
111	Density-Functional Calculations for Ozone: Striking Results for an Important Molecule. Physical Review Letters, 1984, 52, 2002-2005.	2.9	17
112	Energy surfaces of lowâ€lying states of C3. Journal of Chemical Physics, 1985, 82, 5078-5083.	1.2	17
113	Si-H clusters, defects, and hydrogenated silicon. Physical Review B, 2001, 64, .	1.1	17
114	Structure of amorphous Ag/Ge/S alloys: experimentally constrained density functional study. Journal of Physics Condensed Matter, 2015, 27, 485304.	0.7	17
115	Polycarbonate Simulations with a Density Functional Based Force Field. Journal of Physical Chemistry A, 1999, 103, 5387-5398.	1.1	16
116	Density Functional Study of Reactions of Phenoxides with Polycarbonate. Journal of Physical Chemistry A, 2001, 105, 3008-3015.	1.1	16
117	Collective excitations and viscosity in liquid Bi. Journal of Chemical Physics, 2016, 145, 184502.	1.2	16
118	Bonding in phase change materials: concepts and misconceptions. Journal of Physics Condensed Matter, 2018, 30, 153001.	0.7	16
119	Electronic structure of sos - a comparison with O3, SO2, and S3. Chemical Physics Letters, 1986, 125, 221-224.	1.2	15
120	Surface barrier in W(110). I. Self-consistent film calculations. Physical Review B, 1986, 34, 6695-6698.	1.1	15
121	Stability and structure of LinH molecules (n=3â€“6): Experimental and density functional study. Journal of Chemical Physics, 2004, 120, 5128-5132.	1.2	15
122	Density Functional Calculations of ATP Systems. 1. Crystalline ATP Hydrates and Related Molecules. Journal of Physical Chemistry B, 2006, 110, 8110-8120.	1.2	15
123	Density functional study of structure and dynamics in liquid antimony and Sbn clusters. Journal of Chemical Physics, 2017, 146, 194502.	1.2	15
124	Cluster calculations using muffin-tin orbitals. Journal of Physics C: Solid State Physics, 1976, 9, 2739-2748.	1.5	14
125	Surface barrier determination using spin-polarized LEED: W(001). Solid State Communications, 1982, 44, 17-22.	0.9	14
126	Density functional calculations with simulated annealing?isomers of S7X [X ? O, S, Se], Se8, O8. International Journal of Quantum Chemistry, 1990, 38, 141-151.	1.0	14

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127	Density Functional Study of Crystalline Analogs of Polycarbonates. Macromolecules, 1998, 31, 7784-7790.	2.2	14
128	Density functional simulations of structure and polymorphism in Ga/Sb films. Journal of Physics Condensed Matter, 2013, 25, 115801.	0.7	14
129	Speeding up crystallization. Science, 2017, 358, 1386-1386.	6.0	14
130	Density functional calculations for lowâ€lying states of CO2. Journal of Chemical Physics, 1983, 79, 1885-1890.	1.2	13
131	Surface barrier in W(110). II. Low-energy electron diffraction fine-structure analysis. Physical Review B, 1986, 34, 6699-6703.	1.1	13
132	Equilibrium polymerization of cyclic carbonate oligomers. Journal of Chemical Physics, 2001, 115, 3895-3905.	1.2	12
133	Branching Reactions in Polycarbonate:Â A Density Functional Study. Macromolecules, 2003, 36, 1355-1360.	2.2	12
134	Chemisorption and surface barrier structure. Surface Science, 1986, 176, 691-700.	0.8	11
135	Structure of phosphorus clusters by simulated annealing. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 26, 349-351.	1.0	10
136	Molecular Calculations with the Density Functional Formalism. Advances in Chemical Physics, 2007, , 413-437.	0.3	10
137	Equilibrium polymerization of cyclic carbonate oligomers. III. Chain branching and the gel transition. Journal of Chemical Physics, 2002, 117, 6841-6851.	1.2	9
138	The crystal and molecular structure of theÏ€-complex [C₄H₆Co(CO)₂]₂. Zeitschrift FÃ¼r Kristallographie, 1966, 123, 330-337.	1.1	8
139	Aluminum and gallium clusters ? a comparative study using simulated annealing. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 26, 23-27.	1.0	8
140	Die Berechnung von MolekÃ¼lstrukturen durch eine Kombination von Dichtefunktionalâ€•und MolekÃ¼ldynamikmethoden. Angewandte Chemie, 1991, 103, 647-657.	1.6	7
141	Equilibrium polymerization of cyclic carbonate oligomers. II. Role of multiple active sites. Journal of Chemical Physics, 2002, 116, 7724-7732.	1.2	6
142	The chemical bond in solidsâ€”revisited. Journal of Physics Condensed Matter, 2022, 34, 343001.	0.7	6
143	Density Functional Theory: A Personal View. Springer Series in Solid-state Sciences, 2012, , 1-28.	0.3	5
144	Isomers of S7O2: A Simulated Annealing Study. Inorganic Chemistry, 1994, 33, 1340-1343.	1.9	4

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145	Reactions of Polycarbonate with Cyclohexene Oxide and Phosphites:Â A Density Functional Study. Macromolecules, 2002, 35, 2327-2334.	2.2	4
146	Comment on â€œFormation of Large Voids in the Amorphous Phase-Change Memory<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Ge</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi>Sb</mml:mi><mml:mn Physical Review Letters, 2010, 104, 019603; author replly 019604.	2.9	4
147	Tuning electronic properties of graphene heterostructures by amorphous-to-crystalline phase transitions. Physical Review B, 2016, 93, .	1.1	4
148	Density functional and classical simulations of liquid and glassy selenium. Physical Review B, 2020, 102, .	1.1	4
149	Density functional calculations with simulated annealing â€“ clusters and amorphous materials. Physica Scripta, 1991, T35, 154-158.	1.2	4
150	Schwerpunkt '84: Physikalische Forschung mit dem Computer: Das Dichtefunktional â€” die Methode zur Berechnung von Bindungseigenschaften?. Physik Journal, 1984, 40, 149-152.	0.1	3
151	Density functional calculations for polymers and clusters â€“ progress and limitations. Computational Materials Science, 2001, 22, 1-6.	1.4	3
152	Density functional simulations of a conductive bridging random access memory cell: Ag filament formation in amorphous <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>GeS</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mm Physical Review Materials, 2022, 6, .	0.9	3
153	Cluster geometries from density functional calculations â€“ prospects and limitations. European Physical Journal D, 1999, 9, 81-84.	0.6	2
154	Density functional/Monte Carlo study of ring-opening polymerization. Computer Physics Communications, 2002, 147, 325-330.	3.0	2
155	Melt-quenched and as-deposited structures of amorphous selenium: a density functional/ molecular dynamics comparison. Journal of Physics Condensed Matter, 2021, 33, 445401.	0.7	2
156	Theoretical Concepts. Springer Series in Chemical Physics, 1994, , 13-205.	0.2	2
157	Structure and spectroscopy of small atomic clusters. Topics in Current Chemistry, 1996, , 87-118.	4.0	1
158	Exchange-Correlation Energy Functionals in the Density Functional Formalism. , 1984, , 229-243.		1
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160	Density Functional Calculations for Molecules and Clusters â€” Li n , Li n O, C n. , 1998, , 349-360.		1
161	A note on model surface state calculations. Physics Letters, Section A: General, Atomic and Solid State Physics, 1968, 27, 135-136.	0.9	0
162	Reply to â€˜â€˜Comment: On the equilibrium of Hg2 moleculeâ€™â€™. Journal of Chemical Physics, 1985, 83, 2622-2622.	1.2	0

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163	Surface barrier studies with LEED fine structure analysis. Applications of Surface Science, 1985, 22-23, 35-47.	1.0	0
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