Robert O Jones

List of Publications by Citations

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	The density functional formalism, its applications and prospects. *Reviews of Modern Physics*, **1989**, 61, 689-746	40.5	3143
172	Density functional theory: Its origins, rise to prominence, and future. *Reviews of Modern Physics*, **2015**, 87, 897-923	40.5	666
171	The surface energy of a bounded electron gas. *Journal of Physics F: Metal Physics*, **1974**, 4, 1170-1186		406
170	Structural phase transitions on the nanoscale: The crucial pattern in the phase-change materials Ge2Sb2Te5 and GeTe. *Physical Review B*, **2007**, 76,	3.3	373
169	Smallest carbon nanotube is 3 a in diameter. *Physical Review Letters*, **2004**, 92, 125502	7.4	244
168	Surface barrier for electrons in metals. *Physical Review B*, **1988**, 37, 6113-6120	3.3	240
167	Density functional theory and molecular bonding. III. Iron-series dimers. *Journal of Chemical Physics*, **1979**, 70, 830	3.9	233
166	Density Functional Calculations for Atoms, Molecules and Clusters. *Physica Scripta*, **1980**, 21, 394-401	2.6	216
165	From local structure to nanosecond recrystallization dynamics in AgInSbTe phase-change materials. *Nature Materials*, **2011**, 10, 129-34	27	204
164	Electronic band structure and covalency in diamond-type semiconductors. *Journal of Physics C: Solid State Physics*, **1969**, 2, 719-732		200
163	Structure of sulfur clusters using simulated annealing: S2 to S13. *Journal of Chemical Physics*, **1988**, 89, 6823-6835	3.9	198
162	Simulated annealing study of neutral and charged clusters: Aln and Gan. *Journal of Chemical Physics* , **1993**, 99, 1194-1206	3.9	175
161	Surface barrier in metals: A new model with application to W(001). *Physical Review B*, **1984**, 29, 6474-6480	3.3	172
160	Structure of phosphorus clusters using simulated annealing: P2 to P8. *Journal of Chemical Physics*, **1990**, 92, 6710-6721	3.9	168
159	Structure and Bonding in Carbon Clusters C14 to C24: Chains, Rings, Bowls, Plates, and Cages. *Physical Review Letters*, **1997**, 79, 443-446	7.4	163
158	Total-energy differences: Sources of error in local-density approximations. *Physical Review B*, **1985**, 31, 7588-7602	3.3	161
157	Density functional study of carbon clusters C2n (2?n?16). I. Structure and bonding in the neutral clusters. *Journal of Chemical Physics*, **1999**, 110, 5189-5200	3.9	158

156	The structure of selenium clusters Se3 TO Se8. *Chemical Physics Letters*, **1987**, 139, 540-545	2.5	156
155	First-principles molecular-dynamics simulation of liquid and amorphous selenium. *Physical Review B* , **1991**, 43, 3856-3870	3.3	151
154	Molecular bonding in Group IIA dimers Be2Ba2. *Journal of Chemical Physics*, **1979**, 71, 1300-1308	3.9	150
153	Density functional theory and molecular bonding. I. First-row diatomic molecules. *Journal of Chemical Physics*, **1999**, 67, 3970	3.9	135
152	Muffin-tin orbitals and the total energy of atomic clusters. *Physical Review B*, **1977**, 15, 3027-3038	3.3	131
151	Structure and spin in small iron clusters. *Chemical Physics Letters*, **1995**, 233, 632-638	2.5	119
150	Structure and bonding in small aluminum clusters. *Physical Review Letters*, **1991**, 67, 224-227	7.4	117
149	Density functional study of structure and bonding in lithium clusters Lin and their oxides LinO. *Journal of Chemical Physics*, **1997**, 106, 4566-4574	3.9	106
148	Binary alloys of Ge and Te: order, voids, and the eutectic composition. *Physical Review Letters*, **2008**, 100, 205502	7.4	103
147	Density functional study of phosphorus and arsenic clusters using local and nonlocal energy functionals. *Journal of Chemical Physics*, **1994**, 100, 4941-4946	3.9	96
146	Structure of phosphorus clusters using simulated annealing. II. P9, P10, P11, anions P2, P2, P3, and cations P+n to n=11. *Journal of Chemical Physics*, **1992**, 96, 7564-7572	3.9	91
145	Density functional study of amorphous, liquid and crystalline Ge(2)Sb(2)Te(5): homopolar bonds and/or AB alternation?. *Journal of Physics Condensed Matter*, **2008**, 20, 465103	1.8	88
144	ATP Hydrolysis in Water A Density Functional Study. *Journal of Physical Chemistry B*, **2003**, 107, 11774-11783	3.4	86
143	Energy surfaces of low-lying states of O3 and SO2. *Journal of Chemical Physics*, **1985**, 82, 325-332	3.9	84
142	Structure and bonding in mixed siliconcarbon clusters and their anions. *Journal of Chemical Physics* , **1996**, 105, 5048-5060	3.9	81
141	Rings and chains in sulfur cluster anions S to S9Theory (simulated annealing) and experiment (photoelectron detachment). *Journal of Chemical Physics*, **1995**, 102, 5917-5936	3.9	78
140	Dynamical corrections to the image potential. *Journal of Physics C: Solid State Physics*, **1973**, 6, 3585-3604		76
139	Structure and spectroscopy of phosphorus cluster anions: Theory (simulated annealing) and experiment (photoelectron detachment). *Journal of Chemical Physics*, **1995**, 103, 9549-9562	3.9	74

138	LEED fine structure: Origins and applications. *Surface Science Reports*, **1988**, 9, 165-196	12.9	74
137	Experimentally constrained density-functional calculations of the amorphous structure of the prototypical phase-change material Ge2Sb2Te5. *Physical Review B*, **2009**, 80,	3.3	73
136	Carbon species confined inside carbon nanotubes: A density functional study. *Physical Review B*, **2003**, 68,	3.3	73
135	Extensions of the LSD approximation in density functional calculations. *Journal of Chemical Physics*, **1980**, 72, 5357-5362	3.9	71
134	Intrinsic Surface States in Semiconductors. *Physical Review Letters*, **1968**, 20, 992-994	7.4	71
133	Density functional theory of 3d-transition element atoms. *Journal of Chemical Physics*, **1978**, 68, 3316-3317	3.9	68
132	Density functional theory and molecular bonding. II. Alkali dimers. *Journal of Chemical Physics*, **1978**, 68, 1190-1193	3.9	68
131	Low-Energy Electron-Diffraction Intensity Calculations for Beryllium with a Realistic Crystal Potential. *Physical Review B*, **1971**, 3, 3228-3243	3.3	68
130	Nucleus-driven crystallization of amorphous Ge2Sb2Te5: A density functional study. *Physical Review B*, **2012**, 86,	3.3	66
129	Model interatomic potential for simulations in selenium. *Physical Review B*, **1996**, 53, 6165-6173	3.3	65
128	Sulfur and selenium helices: Structure and electronic properties. *Journal of Chemical Physics*, **1988**, 88, 2652-2658	3.9	65
127	Polymorphism in phase-change materials: melt-quenched and as-deposited amorphous structures in Ge2Sb2Te5 from density functional calculations. *Physical Review B*, **2011**, 83,	3.3	64
126	Beyond the method of images□he interaction of charged particles with real surfaces. *Advances in Physics*, **1988**, 37, 341-358	18.4	58
125	Density functional and Monte Carlo studies of sulfur. I. Structure and bonding in Sn rings and chains (n=2□8). *Journal of Chemical Physics*, **2003**, 118, 9257-9265	3.9	57
124	Force calculations in the density functional formalism. *Journal of Chemical Physics*, **1981**, 75, 3904-3908	3.9	57
123	Image force for a moving charge. *Journal of Physics C: Solid State Physics*, **1974**, 7, 3751-3754		56
122	Structure of amorphous Ge8Sb2Te11: GeTe-Sb2Te3 alloys and optical storage. *Physical Review B*, **2009**, 79,	3.3	53
121	Simulation of crystallization in Ge2Sb2Te5: A memory effect in the canonical phase-change material. *Physical Review B*, **2014**, 90,	3.3	51

120	Density functional calculations for H2O, NH3, and CO2 using localized muffin-tin orbitals. *Journal of Chemical Physics*, **1983**, 79, 1874-1884	3.9	50
119	Self-interaction corrections in the density functional formalism. *Solid State Communications*, **1981**, 37, 249-252	1.6	50
118	Polymerization in liquid phosphorus: Simulation of a phase transition. *Physical Review B*, **1994**, 50, 17047-17053	3.3	49
117	Inelastic Effects in Low-Energy Electron Diffraction. *Physical Review Letters*, **1969**, 22, 1186-1188	7.4	49
116	Pseudopotentials in Density-Functional Theory. *Physical Review Letters*, **1978**, 41, 191-194	7.4	48
115	Low-Energy Electron-Diffraction Intensity Calculations with a Realistic Crystal Potential. *Physical Review Letters*, **1970**, 25, 516-520	7.4	46
114	Density functional study of crystalline polyethylene. *Chemical Physics Letters*, **1997**, 272, 347-352	2.5	45
113	Surface representations and complex band structure of a diamond-type semiconductor. *Proceedings of the Physical Society*, **1966**, 89, 443-451		44
112	Anisotropic thermal expansion in silicates: A density functional study of □eucryptite and related materials. *Physical Review B*, **2000**, 62, 11487-11493	3.3	43
111	Crystallization processes in the phase change material Ge2Sb2Te5: Unbiased density functional/molecular dynamics simulations. *Physical Review B*, **2016**, 94,	3.3	40
110	Density variations in liquid tellurium: Roles of rings, chains, and cavities. *Physical Review B*, **2010**, 81,	3.3	40
109	Structure and dynamics in amorphous tellurium and Ten clusters: A density functional study. *Physical Review B*, **2012**, 85,	3.3	40
108	Multiplet structure and charge distributions in silicon and germanium dimers. *Physical Review A*, **1978**, 18, 2159-2166	2.6	40
107	Bonding trends in the group-IVA dimers C2-Pb2. *Physical Review A*, **1979**, 19, 1813-1818	2.6	39
106	Amorphous Ge□Te□density functional, high-energy x-ray and neutron diffraction study. *Journal of Physics Condensed Matter*, **2012**, 24, 015802	1.8	38
105	Density functional study of molecular crystals: Polyethylene and a crystalline analog of bisphenol-A polycarbonate. *Journal of Chemical Physics*, **1998**, 108, 6947-6951	3.9	38
104	Anisotropic thermal expansion in the silicate □eucryptite: A neutron diffraction and density functional study. *Physical Review B*, **1998**, 58, 6219-6223	3.3	38
103	Geometric and electronic structure of clusters. *Zeitschrift F□ Physik D-Atoms Molecules and Clusters* , **1991**, 20, 77-80		38

102	Structure, electronic, and vibrational properties of glassy Ga11Ge11Te78: Experimentally constrained density functional study. *Physical Review B*, **2012**, 86,	3.3	36
101	Structure, bonding, and dynamics in heterocyclic sulfur-selenium molecules, SexSy. *Journal of the American Chemical Society*, **1990**, 112, 2590-2596	16.4	36
100	Energy differences using an accurate local density functional. *Journal of Chemical Physics*, **1982**, 76, 3098-3101	3.9	36
99	Cluster calculations of the electronic structure of transition metal surfaces. *Surface Science*, **1975**, 53, 409-428	1.8	35
98	Density-functional formalism: Sources of error in local-density approximations. *Physical Review Letters*, **1985**, 55, 107-110	7.4	33
97	Molecular bonding in LiBe, LiMg, and LiCa. *Journal of Chemical Physics*, **1980**, 72, 3197-3200	3.9	33
96	Energy surfaces for Si3 and C3: A comparative study. *Physical Review A*, **1985**, 32, 2589-2594	2.6	32
95	Low-lying states of thiozone, S3. *Journal of Chemical Physics*, **1986**, 84, 318-322	3.9	31
94	Energy surfaces of polymeric sulfur: Structure and electronic properties. *Physical Review Letters*, **1986**, 57, 1145-1148	7.4	30
93	Fine-structure analysis of spin-polarized low-energy electron diffraction from W(001). *Physical Review B*, **1983**, 27, 4702-4711	3.3	29
92	Model calculation of surface states in silicon. *Journal of Physics C: Solid State Physics*, **1972**, 5, 1615-1628		29
91	Density functional study of carbonic acid clusters. *Journal of Chemical Physics*, **2000**, 112, 6571-6575	3.9	27
90	Amorphous phosphorus: A cluster-network model. *Physical Review B*, **1992**, 45, 8995-9005	3.3	27
89	Energy surfaces and structure of S7O. *Journal of the American Chemical Society*, **1989**, 111, 825-828	16.4	27
88	Low-energy-electron-diffraction fine structure in W(001) for energies from 0 to 35 eV. *Physical Review B*, **1985**, 32, 6131-6137	3.3	27
87	A reactive force field simulation of liquid-liquid phase transitions in phosphorus. *Journal of Chemical Physics*, **2004**, 121, 8147-57	3.9	26
86	Density functional calculations of ATP systems. 2. ATP hydrolysis at the active site of actin. *Journal of Physical Chemistry B*, **2006**, 110, 8121-9	3.4	25
85	Amorphous structures of Ge/Sb/Te alloys: Density functional simulations. *Physica Status Solidi (B): Basic Research*, **2012**, 249, 1851-1860	1.3	24

84	Density Functional Study of Polycarbonate. 2. Crystalline Analogs, Cyclic Oligomers, and Their Fragments. *Macromolecules*, **1999**, 32, 3396-3404	5.5	22
83	Electronic structure of stepped transition metal surfaces. *Journal of Physics C: Solid State Physics*, **1975**, 8, L199-L202		22
82	Structure of liquid phase change material AgInSbTe from density functional/molecular dynamics simulations. *Applied Physics Letters*, **2009**, 94, 251905	3.4	21
81	Cage molecules containing elements of groups V and VI. II. Molecular dynamics study of P4S3 and P3□. *Journal of Chemical Physics*, **1992**, 96, 2951-2952	3.9	21
80	Spin-polarization in LEED: A comparison of theoretical predictions. *Surface Science*, **1976**, 61, 307-316	1.8	21
79	Prediction and observation of ring and chain isomers in Sn□ ons. *Chemical Physics Letters*, **1995**, 236, 43-49	2.5	20
78	Cage molecules containing elements of groups V and VI. I. Structure determinations using simulated annealing. *Journal of Chemical Physics*, **1992**, 96, 2942-2950	3.9	20
77	Molecular Structures from Density Functional Calculations with Simulated Annealing. *Angewandte Chemie International Edition in English*, **1991**, 30, 630-640		19
76	First principles MD simulation of liquid and amorphous selenium. *Journal of Non-Crystalline Solids*, **1990**, 117-118, 922-925	3.9	19
75	Spin-dependent features in leed intensity curves. *Surface Science*, **1978**, 71, 101-106	1.8	19
74	Intensities of Low-Energy-Electron-Diffraction Beams from Be(0001). *Physical Review B*, **1972**, 6, 407-416	3.3	19
73	Density functional study of polypropylene and its submolecules. *Journal of Chemical Physics*, **1997**, 106, 8545-8551	3.9	18
72	Structure and dynamics in liquid bismuth and Bi(n) clusters: a density functional study. *Journal of Chemical Physics*, **2014**, 141, 194503	3.9	17
71	Catalytic Reactions of Living Polymers: Density Functional Study of Reactivity of Phenol and Phenoxides with the Cyclic Tetramer of Polycarbonate. *Journal of Physical Chemistry A*, **2000**, 104, 2793-2798	2.8	17
70	Energy surfaces of low-lying states of C3. *Journal of Chemical Physics*, **1985**, 82, 5078-5083	3.9	17
69	Local densities of states and bonding properties of 3d-transition metal clusters. *Surface Science*, **1976**, 61, 255-271	1.8	17
68	Density functional and Monte Carlo studies of sulfur. II. Equilibrium polymerization of the liquid phase. *Journal of Chemical Physics*, **2003**, 119, 8704-8715	3.9	16
67	Si-H clusters, defects, and hydrogenated silicon. *Physical Review B*, **2001**, 64,	3.3	16

66	Density-Functional Calculations for Ozone: Striking Results for an Important Molecule. *Physical Review Letters*, **1984**, 52, 2002-2005	7.4	16
65	On the existence of Stark ladders in finite crystals. *Journal of Physics C: Solid State Physics*, **1972**, 5, 2149-2155		16
64	Crystallization of supercooled liquid antimony: A density functional study. *Physical Review B*, **2017**, 96,	3.3	15
63	Polycarbonate Simulations with a Density Functional Based Force Field. *Journal of Physical Chemistry A*, **1999**, 103, 5387-5398	2.8	15
62	Electronic structure of sos - a comparison with O3, SO2, and S3. *Chemical Physics Letters*, **1986**, 125, 221-224	2.3	15
61	Surface barrier in W(110). I. Self-consistent film calculations. *Physical Review B*, **1986**, 34, 6695-6698	3.3	15
60	Density functional calculations of ATP systems. 1. Crystalline ATP hydrates and related molecules. *Journal of Physical Chemistry B*, **2006**, 110, 8110-20	3.4	14
59	Stability and structure of Li(n)H molecules (n=3-6): experimental and density functional study. *Journal of Chemical Physics*, **2004**, 120, 5128-32	3.9	14
58	Density Functional Study of Reactions of Phenoxides with Polycarbonate. *Journal of Physical Chemistry A*, **2001**, 105, 3008-3015	2.8	14
57	Density Functional Study of Crystalline Analogs of Polycarbonates. *Macromolecules*, **1998**, 31, 7784-7790	5.5	14
56	Surface barrier determination using spin-polarized LEED: W(001). *Solid State Communications*, **1982**, 44, 17-22	1.6	14
55	Structure, electronic, and vibrational properties of amorphous AsS2 and AgAsS2: Experimentally constrained density functional study. *Physical Review B*, **2014**, 89,	3.3	13
54	Surface barrier in W(110). II. Low-energy electron diffraction fine-structure analysis. *Physical Review B*, **1986**, 34, 6699-6703	3.3	13
53	Density functional calculations for low-lying states of CO2. *Journal of Chemical Physics*, **1983**, 79, 1885-1890	3.9	13
52	Cluster calculations using muffin-tin orbitals. *Journal of Physics C: Solid State Physics*, **1976**, 9, 2739-2748		13
51	Phase change memory materials: Rationalizing the dominance of Ge/Sb/Te alloys. *Physical Review B* , **2020**, 101,	3.3	13
50	Speeding up crystallization. *Science*, **2017**, 358, 1386	33.3	12
49	Equilibrium polymerization of cyclic carbonate oligomers. *Journal of Chemical Physics*, **2001**, 115, 3895-3905	3.9	12

48	Density functional calculations with simulated annealing□somers of S7X [X ? O, S, Se], Se8, O8. *International Journal of Quantum Chemistry*, **1990**, 38, 141-151	2.1	12
47	Collective excitations and viscosity in liquid Bi. *Journal of Chemical Physics*, **2016**, 145, 184502	3.9	12
46	Structure of amorphous Ag/Ge/S alloys: experimentally constrained density functional study. *Journal of Physics Condensed Matter*, **2015**, 27, 485304	1.8	11
45	Chemisorption and surface barrier structure. *Surface Science*, **1986**, 176, 691-700	1.8	11
44	Bonding in phase change materials: concepts and misconceptions. *Journal of Physics Condensed Matter*, **2018**, 30, 153001	1.8	10
43	Density functional simulations of structure and polymorphism in Ga/Sb films. *Journal of Physics Condensed Matter*, **2013**, 25, 115801	1.8	10
42	Molecular Calculations with the Density Functional Formalism. *Advances in Chemical Physics*, **2007**, 413-437		10
41	Branching Reactions in Polycarbonate: A Density Functional Study. *Macromolecules*, **2003**, 36, 1355-1360	5.5	10
40	Equilibrium polymerization of cyclic carbonate oligomers. III. Chain branching and the gel transition. *Journal of Chemical Physics*, **2002**, 117, 6841-6851	3.9	9
39	Structure of phosphorus clusters by simulated annealing. *Zeitschrift F□ Physik D-Atoms Molecules and Clusters*, **1993**, 26, 349-351		9
38	Aluminum and gallium clusters □a comparative study using simulated annealing. *Zeitschrift F□ Physik D-Atoms Molecules and Clusters*, **1993**, 26, 23-27		8
37	Density functional study of structure and dynamics in liquid antimony and Sb clusters. *Journal of Chemical Physics*, **2017**, 146, 194502	3.9	7
36	Die Berechnung von Molek□strukturen durch eine Kombination von Dichtefunktional- und Molek□dynamikmethoden. *Angewandte Chemie*, **1991**, 103, 647-657	3.6	7
35	The crystal and molecular structure of the □complex [C4H6Co(CO)2]2. *Zeitschrift F□ Kristallographie*, **1966**, 123, 330-337		7
34	Equilibrium polymerization of cyclic carbonate oligomers. II. Role of multiple active sites. *Journal of Chemical Physics*, **2002**, 116, 7724-7732	3.9	6
33	Density Functional Theory: A Personal View. *Springer Series in Solid-state Sciences*, **2012**, 1-28	0.4	5
32	Tuning electronic properties of graphene heterostructures by amorphous-to-crystalline phase transitions. *Physical Review B*, **2016**, 93,	3.3	4
31	Comment on "Formation of large voids in the amorphous phase-change memory Ge2Sb2Te5 alloy". *Physical Review Letters*, **2010**, 104, 019603; author replly 019604	7.4	4

30	Reactions of Polycarbonate with Cyclohexene Oxide and Phosphites: A Density Functional Study. *Macromolecules*, **2002**, 35, 2327-2334	5.5	4
29	Density functional calculations with simulated annealing clusters and amorphous materials. *Physica Scripta*, **1991**, T35, 154-158	2.6	4
28	Density functional calculations for polymers and clusters progress and limitations. *Computational Materials Science*, **2001**, 22, 1-6	3.2	3
27	Schwerpunkt '84: Physikalische Forschung mit dem Computer: Das Dichtefunktional die Methode zur Berechnung von Bindungseigenschaften?. *Physik Journal*, **1984**, 40, 149-152		3
26	Density functional/Monte Carlo study of ring-opening polymerization. *Computer Physics Communications*, **2002**, 147, 325-330	4.2	2
25	Cluster geometries from density functional calculations prospects and limitations. *European Physical Journal D*, **1999**, 9, 81-84	1.3	2
24	Isomers of S7O2: A Simulated Annealing Study. *Inorganic Chemistry*, **1994**, 33, 1340-1343	5.1	2
23	Theoretical Concepts. *Springer Series in Chemical Physics*, **1994**, 13-205	0.3	2
22	Density functional and classical simulations of liquid and glassy selenium. *Physical Review B*, **2020**, 102,	3.3	2
21	Exchange-Correlation Energy Functionals in the Density Functional Formalism **1984**, 229-243		1
20	Simulated Annealing Studies of Sulphur and Selenium Clusters. *Springer Proceedings in Physics*, **1990**, 214-231	0.2	1
19	Density Functional Calculations for Molecules and Clusters Lin, LinO, Cn **1998**, 349-360		1
18	Structure and spectroscopy of small atomic clusters. *Topics in Current Chemistry*, **1996**, 87-118		1
17	Molecular calculations using the muffin-tin orbital method. *International Journal of Quantum Chemistry*, **2009**, 12, 71-74	2.1	
16	Ring-Opening and Branching in Polycarbonates: A Density Functional-Monte Carlo Study. *ACS Symposium Series*, **2005**, 200-213	0.4	
15	A Combined Density Functional and Monte Carlo Study of Polycarbonate. *Materials Research Society Symposia Proceedings*, **2001**, 677, 311		
14	Density Functional Calculations - A Database for Parameterizing Interatomic Potentials **1991**, 437-450		
13	Reply to comment: On the equilibrium of Hg2 molecule *Journal of Chemical Physics*, **1985**, 83, 2622-2623	3.9	

List of Publications

12	Surface barrier studies with LEED fine structure analysis. *Applications of Surface Science*, **1985**, 22-23, 35-47	
11	A note on model surface state calculations. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **1968**, 27, 135-136	2.3
10	Structure and bonding in aluminium and gallium clusters **1992**, 305-311	
9	Density Functional Calculations with Simulated Annealing New Perspectives for Molecular Calculations **1990**, 127-142	
8	Geometric and electronic structure of clusters **1991**, 527-530	
7	Structural Trends in Clusters and Disordered Systems. *Springer Series in Solid-state Sciences*, **1993**, 67-76	0.4
6	Density Functionals, Molecular Dynamics, and More **1995**, 37-66	
5	Molecules and Molecular Dynamics. *NATO ASI Series Series B: Physics*, **1995**, 273-297	
4	Cluster geometries from density functional calculations prospects and limitations **1999**, 81-84	
3	The Prototype Phase Change Material ({mathrm{Ge}_2}{mathrm{Sb}_2}{mathrm{Te}_5}): Amorphous Structure and Crystallization. *Springer Series in Materials Science*, **2015**, 457-484	0.9
2	Density Functional Calculations for Atomic Clusters **1979**, 55-70	
1	Density-functional formalism: Vxc, discontinuities, and the local density approximation. *Lecture Notes in Physics*, **1987**, 77-92	0.8