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	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 Physical Review Materials, 2022, 6, .	0.9	3
2	The chemical bond in solidsâ€”revisited. Journal of Physics Condensed Matter, 2022, 34, 343001.	0.7	6
3	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
4	Density functional and classical simulations of liquid and glassy selenium. Physical Review B, 2020, 102, .	1.1	4
5	Phase change memory materials: Rationalizing the dominance of Ge/Sb/Te alloys. Physical Review B, 2020, 101, .	1.1	22
6	Bonding in phase change materials: concepts and misconceptions. Journal of Physics Condensed Matter, 2018, 30, 153001.	0.7	16
7	pyMolDyn: Identification, structure, and properties of cavities/vacancies in condensed matter and molecules. Journal of Computational Chemistry, 2017, 38, 389-394.	1.5	42
8	Speeding up crystallization. Science, 2017, 358, 1386-1386.	6.0	14
9	Crystallization of supercooled liquid antimony: A density functional study. Physical Review B, 2017, 96, .	1.1	20
10	Density functional study of structure and dynamics in liquid antimony and Sbn clusters. Journal of Chemical Physics, 2017, 146, 194502.	1.2	15
11	Collective excitations and viscosity in liquid Bi. Journal of Chemical Physics, 2016, 145, 184502.	1.2	16
12	Tuning electronic properties of graphene heterostructures by amorphous-to-crystalline phase transitions. Physical Review B, 2016, 93, .	1.1	4
13	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
14	Structure of amorphous Ag/Ge/S alloys: experimentally constrained density functional study. Journal of Physics Condensed Matter, 2015, 27, 485304.	0.7	17
15	Density functional theory: Its origins, rise to prominence, and future. Reviews of Modern Physics, 2015, 87, 897-923.	16.4	962
16	The Prototype Phase Change Material $${mathrm{Ge}_2}{mathrm{Sb}_2}{mathrm{Te}_5}$$ Ge 2 Sb 2 Te 5 : Amorphous Structure and Crystallization. Springer Series in Materials Science, 2015, , 457-484.	0.4	0
17	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:mi mathvariant="normal">Te</mml:mi><mml:mn>5</mml:mn></mml:math>: A memory effect in	1.1	68
18	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> <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mtext>Ag</mml:mtext><mml:msub><mml:mtext>AsS</mml:mtext><mml:mn> Experimentally constrained density functional study. Physical Review B, 2014, 89, .	1.1	18

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19	Structure and dynamics in liquid bismuth and Bin clusters: A density functional study. Journal of Chemical Physics, 2014, 141, 194503.	1.2	21
20	Density functional simulations of structure and polymorphism in Ga/Sb films. Journal of Physics Condensed Matter, 2013, 25, 115801.	0.7	14
21	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
22	Nucleus-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: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 />	1.1	79
23		1.1	41
24	Amorphous Ge₁₅Te₈₅: density functional, high-energy x-ray and neutron diffraction study. Journal of Physics Condensed Matter, 2012, 24, 015802.	0.7	43
25	Amorphous structures of Ge/Sb/Te alloys: Density functional simulations. Physica Status Solidi (B): Basic Research, 2012, 249, 1851-1860.	0.7	25
26	Density Functional Theory: A Personal View. Springer Series in Solid-state Sciences, 2012, , 1-28.	0.3	5
27	From local structure to nanosecond recrystallization dynamics in AgInSbTeÂphase-changeÂmaterials. Nature Materials, 2011, 10, 129-134.	13.3	238
28	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 />	1.1	75
29	Comment on âceFormation 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:mi> Physical Review Letters, 2010, 104, 019603; author reply 019604.	2.9	4
30	Density variations in liquid tellurium: Roles of rings, chains, and cavities. Physical Review B, 2010, 81, .	1.1	48
31	Structure of amorphousGe8Sb2Te11:GeTe-Sb2Te3alloys and optical storage. Physical Review B, 2009, 79, .	1.1	58
32	Structure of liquid phase change material AgInSbTe from density functional/molecular dynamics simulations. Applied Physics Letters, 2009, 94, 251905.	1.5	23
33	Experimentally constrained density-functional calculations of the amorphous structure of the prototypical phase-change materialGe2Sb2Te5. Physical Review B, 2009, 80, .	1.1	77
34	Molecular calculations using the muffin-tin orbital method. International Journal of Quantum Chemistry, 2009, 12, 71-74.	1.0	0
35	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
36	Binary Alloys of Ge and Te: Order, Voids, and the Eutectic Composition. Physical Review Letters, 2008, 100, 205502.	2.9	110

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37	al 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 C	1.1	417
38	Molecular Calculations with the Density Functional Formalism. Advances in Chemical Physics, 2007, , 413-437.	0.3	10
39	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
40	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
41	Ring-Opening and Branching in Polycarbonates: A Density Functional-Monte Carlo Study. ACS Symposium Series, 2005, , 200-213.	0.5	0
42	A reactive force field simulation of liquidâ€“liquid phase transitions in phosphorus. Journal of Chemical Physics, 2004, 121, 8147.	1.2	31
43	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
44	Smallest Carbon Nanotube Is3â€‰â€‰Ã…in Diameter. Physical Review Letters, 2004, 92, 125502.	2.9	272
45	ATP Hydrolysis in Water â^' A Density Functional Study. Journal of Physical Chemistry B, 2003, 107, 11774-11783.	1.2	97
46	Branching Reactions in Polycarbonate:Â A Density Functional Study. Macromolecules, 2003, 36, 1355-1360.	2.2	12
47	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
48	Carbon species confined inside carbon nanotubes:â€ƒA density functional study. Physical Review B, 2003, 68, .	1.1	79
49	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
50	Equilibrium polymerization of cyclic carbonate oligomers. III. Chain branching and the gel transition. Journal of Chemical Physics, 2002, 117, 6841-6851.	1.2	9
51	Equilibrium polymerization of cyclic carbonate oligomers. II. Role of multiple active sites. Journal of Chemical Physics, 2002, 116, 7724-7732.	1.2	6
52	Reactions of Polycarbonate with Cyclohexene Oxide and Phosphites:Â A Density Functional Study. Macromolecules, 2002, 35, 2327-2334.	2.2	4
53	Density functional/Monte Carlo study of ring-opening polymerization. Computer Physics Communications, 2002, 147, 325-330.	3.0	2
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57	A Combined Density Functional and Monte Carlo Study of Polycarbonate. Materials Research Society Symposia Proceedings, 2001, 677, 311.	0.1	0
58	Si-H clusters, defects, and hydrogenated silicon. Physical Review B, 2001, 64, .	1.1	17
59	Anisotropic thermal expansion in silicates: A density functional study ofÎ²-eucryptite and related materials. Physical Review B, 2000, 62, 11487-11493.	1.1	53
60	Density functional study of carbonic acid clusters. Journal of Chemical Physics, 2000, 112, 6571-6575.	1.2	27
61	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
62	Density functional theory and molecular bonding. I. First-row diatomic molecules. Journal of Chemical Physics, 1999, 67, 3970.	1.2	139
63	Cluster geometries from density functional calculations â€“ prospects and limitations. European Physical Journal D, 1999, 9, 81-84.	0.6	2
64	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
65	Density Functional Study of Polycarbonate. 2. Crystalline Analogs, Cyclic Oligomers, and Their Fragments. Macromolecules, 1999, 32, 3396-3404.	2.2	23
66	Polycarbonate Simulations with a Density Functional Based Force Field. Journal of Physical Chemistry A, 1999, 103, 5387-5398.	1.1	16
67	Cluster geometries from density functional calculations â€” prospects and limitations. , 1999, , 81-84.		0
68	Density Functional Study of Crystalline Analogs of Polycarbonates. Macromolecules, 1998, 31, 7784-7790.	2.2	14
69	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
70	Anisotropic thermal expansion in the silicateÎ²-eucryptite: A neutron diffraction and density functional study. Physical Review B, 1998, 58, 6219-6223.	1.1	49
71	Density Functional Calculations for Molecules and Clusters â€” Li n , Li n O, C n. , 1998, , 349-360.		1
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74	Structure and Bonding in Carbon ClustersC14toC24: Chains, Rings, Bowls, Plates, and Cages. Physical Review Letters, 1997, 79, 443-446.	2.9	167
75	Density functional study of crystalline polyethylene. Chemical Physics Letters, 1997, 272, 347-352.	1.2	47
76	Structure and bonding in mixed siliconâ€“carbon clusters and their anions. Journal of Chemical Physics, 1996, 105, 5048-5060.	1.2	83
77	Model interatomic potential for simulations in selenium. Physical Review B, 1996, 53, 6165-6173.	1.1	79
78	Structure and spectroscopy of small atomic clusters. Topics in Current Chemistry, 1996, , 87-118.	4.0	1
79	Structure and spin in small iron clusters. Chemical Physics Letters, 1995, 233, 632-638.	1.2	122
80	Prediction and observation of ring and chain isomers in Snâ¯ i ons. Chemical Physics Letters, 1995, 236, 43-49.	1.2	22
81	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
82	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
83	Density Functionals, Molecular Dynamics, and More. , 1995, , 37-66.		0
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85	Polymerization in liquid phosphorus: Simulation of a phase transition. Physical Review B, 1994, 50, 17047-17053.	1.1	51
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87	Isomers of S7O2: A Simulated Annealing Study. Inorganic Chemistry, 1994, 33, 1340-1343.	1.9	4
88	Theoretical Concepts. Springer Series in Chemical Physics, 1994, , 13-205.	0.2	2
89	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
90	Structure of phosphorus clusters by simulated annealing. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 26, 349-351.	1.0	10

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91	Simulated annealing study of neutral and charged clusters: Alnand Gan. Journal of Chemical Physics, 1993, 99, 1194-1206.	1.2	193
92	Structural Trends in Clusters and Disordered Systems. Springer Series in Solid-state Sciences, 1993, , 67-76.	0.3	0
93	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
94	Amorphous phosphorus: A cluster-network model. Physical Review B, 1992, 45, 8995-9005.	1.1	28
95	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
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98	Density Functional Calculations - A Database for Parameterizing Interatomic Potentials. , 1991, , 437-450.		0
99	Structure and bonding in small aluminum clusters. Physical Review Letters, 1991, 67, 224-227.	2.9	124
100	Molecular Structures from Density Functional Calculations with Simulated Annealing. Angewandte Chemie International Edition in English, 1991, 30, 630-640.	4.4	21
101	Die Berechnung von MolekÃ¼lstrukturen durch eine Kombination von Dichtefunktionalâ€•und MolekÃ¼ldynamikmethoden. Angewandte Chemie, 1991, 103, 647-657.	1.6	7
102	Geometric and electronic structure of clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1991, 20, 77-80.	1.0	40
103	Density functional calculations with simulated annealing â€“ clusters and amorphous materials. Physica Scripta, 1991, T35, 154-158.	1.2	4
104	Geometric and electronic structure of clusters. , 1991, , 527-530.		0
105	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
106	Structure, bonding, and dynamics in heterocyclic sulfur-selenium molecules, SexSy. Journal of the American Chemical Society, 1990, 112, 2590-2596.	6.6	40
107	First principles MD simulation of liquid and amorphous selenium. Journal of Non-Crystalline Solids, 1990, 117-118, 922-925.	1.5	20
108	Structure of phosphorus clusters using simulated annealingâ€”P2 to P8. Journal of Chemical Physics, 1990, 92, 6710-6721.	1.2	188

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109	Simulated Annealing Studies of Sulphur and Selenium Clusters. Springer Proceedings in Physics, 1990, , 214-231.	0.1	1
110	Density Functional Calculations with Simulated Annealing â€" New Perspectives for Molecular Calculations. , 1990, , 127-142.		0
111	Energy surfaces and structure of S7O. Journal of the American Chemical Society, 1989, 111, 825-828.	6.6	31
112	The density functional formalism, its applications and prospects. Reviews of Modern Physics, 1989, 61, 689-746.	16.4	3,538
113	LEED fine structure: Origins and applications. Surface Science Reports, 1988, 9, 165-196.	3.8	78
114	Sulfur and selenium helices: Structure and electronic properties. Journal of Chemical Physics, 1988, 88, 2652-2658.	1.2	69
115	Structure of sulfur clusters using simulated annealing: S2to S13. Journal of Chemical Physics, 1988, 89, 6823-6835.	1.2	214
116	Beyond the method of imagesâ€"the interaction of charged particles with real surfaces. Advances in Physics, 1988, 37, 341-358.	35.9	62
117	Surface barrier for electrons in metals. Physical Review B, 1988, 37, 6113-6120.	1.1	256
118	The structure of selenium clusters â€" Se3 TO Se8. Chemical Physics Letters, 1987, 139, 540-545.	1.2	166
119	Density-functional formalism: V xc, discontinuities, and the local density approximation. Lecture Notes in Physics, 1987, , 77-92.	0.3	0
120	Energy Surfaces of Polymeric Sulfur: Structure and Electronic Properties. Physical Review Letters, 1986, 57, 1145-1148.	2.9	34
121	Chemisorption and surface barrier structure. Surface Science, 1986, 176, 691-700.	0.8	11
122	Electronic structure of sos - a comparison with O3, SO2, and S3. Chemical Physics Letters, 1986, 125, 221-224.	1.2	15
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125	Surface barrier in W(110). II. Low-energy electron diffraction fine-structure analysis. Physical Review B, 1986, 34, 6699-6703.	1.1	13
126	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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128	Energy surfaces forSi3andC3: A comparative study. Physical Review A, 1985, 32, 2589-2594.	1.0	32
129	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
130	Total-energy differences: Sources of error in local-density approximations. Physical Review B, 1985, 31, 7588-7602.	1.1	169
131	Density-functional formalism: Sources of error in local-density approximations. Physical Review Letters, 1985, 55, 107-110.	2.9	37
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137	Exchange-Correlation Energy Functionals in the Density Functional Formalism. , 1984, , 229-243.		1
138	Fine-structure analysis of spin-polarized low-energy electron diffraction from W(001). Physical Review B, 1983, 27, 4702-4711.	1.1	31
139	Density functional calculations for H2O, NH3, and CO2 using localized muffinâ€tin orbitals. Journal of Chemical Physics, 1983, 79, 1874-1884.	1.2	52
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142	Surface barrier determination using spin-polarized LEED: W(001). Solid State Communications, 1982, 44, 17-22.	0.9	14
143	Self-interaction corrections in the density functional formalism. Solid State Communications, 1981, 37, 249-252.	0.9	51
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146	Molecular bonding in LiBe, LiMg, and LiCa. Journal of Chemical Physics, 1980, 72, 3197-3200.	1.2	36
147	Extensions of the LSD approximation in density functional calculations. Journal of Chemical Physics, 1980, 72, 5357-5362.	1.2	74
148	Bonding trends in the group-IVAdimersC2-Pb2. Physical Review A, 1979, 19, 1813-1818.	1.0	42
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151	Density Functional Calculations for Atomic Clusters. , 1979, , 55-70.		0
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155	Pseudopotentials in Density-Functional Theory. Physical Review Letters, 1978, 41, 191-194.	2.9	48
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158	Spin-polarization in LEED: A comparison of theoretical predictions. Surface Science, 1976, 61, 307-316.	0.8	23
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