Stewart Clark

List of Publications by Year
in descending order

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199 papers	31,477 citations	34016 52 h-index	4101 175 g-index
206 all docs	206 docs citations	206 times ranked	26938 citing authors

#	Article	IF	Citations
1	First principles methods using CASTEP. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.4	9,458
2	First-principles simulation: ideas, illustrations and the CASTEP code. Journal of Physics Condensed Matter, 2002, 14, 2717-2744.	0.7	8,382
3	High sensitivity mapping of methylated cytosines. Nucleic Acids Research, 1994, 22, 2990-2997.	6.5	1,749
4	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
5	Variational density-functional perturbation theory for dielectrics and lattice dynamics. Physical Review B, 2006, 73, .	1.1	735
6	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î²</mml:mi></mml:math>phase and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î³</mml:mi><mml:mtext>â€’</mml:mtext><mml:mi>Î²</mml:mi></mml:mrow></mml:math>me transition in multiferroic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Bi</mml:mi><mml:mi mathvariant="norm	1.1	604
7	Defect energy levels in HfO2 high-dielectric-constant gate oxide. Applied Physics Letters, 2005, 87, 183505.	1.5	459
8	Structure and elasticity of MgO at high pressure. American Mineralogist, 1997, 82, 51-60.	0.9	407
9	Band gap and Schottky barrier heights of multiferroic BiFeO3. Applied Physics Letters, 2007, 90, 132903.	1.5	364
10	CpNpG methylation in mammalian cells. Nature Genetics, 1995, 10, 20-27.	9.4	259
11	Limits to doping in oxides. Physical Review B, 2011, 83, .	1.1	248
12	Intrinsic defects in ZnO calculated by screened exchange and hybrid density functionals. Physical Review B, 2010, 81, .	1.1	244
13	Density functional theory in the solid state. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130270.	1.6	242
14	Structure and properties of silicon XII: A complex tetrahedrally bonded phase. Physical Review B, 1995, 52, 4072-4085.	1.1	230
15	Effect of High Pressure on the Crystal Structures of Polymorphs of Glycine. Crystal Growth and Design, 2005, 5, 1415-1427.	1.4	221
16	Band gaps and defect levels in functional oxides. Thin Solid Films, 2006, 496, 1-7.	0.8	218
17	Electron and vibrational spectroscopies using DFT, plane waves and pseudopotentials: CASTEP implementation. Computational and Theoretical Chemistry, 2010, 954, 22-35.	1.5	205
18	Screened exchange density functional applied to solids. Physical Review B, 2010, 82, .	1.1	189

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19	Nature of the electronic band gap in lanthanide oxides. Physical Review B, 2013, 87, .	1.1	182
20	Areneâ€“perfluoroarene interactions in crystal engineering 8: structures of 1â^¶1 complexes of hexafluorobenzene with fused-ring polyaromatic hydrocarbons. New Journal of Chemistry, 2002, 26, 1740-1746.	1.4	181
21	Sp1 binding is inhibited by mCpmCpG methylation. Gene, 1997, 195, 67-71.	1.0	172
22	Structural basis for complement factor Hâ€“linked age-related macular degeneration. Journal of Experimental Medicine, 2007, 204, 2277-2283.	4.2	168
23	Band gap modification of single-walled carbon nanotube and boron nitride nanotube under a transverse electric field. Nanotechnology, 2004, 15, 1837-1843.	1.3	159
24	Precise ab-initio prediction of terahertz vibrational modes in crystalline systems. Chemical Physics Letters, 2007, 442, 275-280.	1.2	157
25	Elastic properties of orthorhombic MgSiO₃perovskite at lower mantle pressures. American Mineralogist, 1997, 82, 635-638.	0.9	143
26	Passivation of oxygen vacancy states in HfO2 by nitrogen. Journal of Applied Physics, 2006, 99, 044105.	1.1	137
27	Practical methods inab initiolattice dynamics. Journal of Physics Condensed Matter, 1997, 9, 7861-7872.	0.7	127
28	Oxygen vacancy levels and electron transport in Al2O3. Applied Physics Letters, 2010, 96, 032905.	1.5	119
29	Defect states in the high-dielectric-constant gate oxide LaAlO3. Applied Physics Letters, 2006, 89, 022907.	1.5	116
30	Structure and electronic properties ofFeSi2. Physical Review B, 1998, 58, 10389-10393.	1.1	110
31	Energy levels of oxygen vacancies in BiFeO3 by screened exchange. Applied Physics Letters, 2009, 94, .	1.5	108
32	High-pressure polymorphism in L-cysteine: the crystal structures of L-cysteine-III and L-cysteine-IV. Acta Crystallographica Section B: Structural Science, 2006, 62, 296-309.	1.8	103
33	Arene-perfluoroarene interactions in crystal engineering: structural preferences in polyfluorinated tolans. Journal of Materials Chemistry, 2004, 14, 413-420.	6.7	101
34	Behavior of hydrogen in wide band gap oxides. Journal of Applied Physics, 2007, 102, .	1.1	99
35	Structural, electronic and vibrational properties of tetragonal zirconia under pressure: a density functional theory study. Journal of Physics Condensed Matter, 2009, 21, 485404.	0.7	97
36	Complex Low Energy Tetrahedral Polymorphs of Group IV Elements from First Principles. Physical Review Letters, 2018, 121, 175701.	2.9	95

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37	Band structure of functional oxides by screened exchange and the weighted density approximation. Physica Status Solidi (B): Basic Research, 2006, 243, 2054-2070.	0.7	88
38	Calculation of point defects in rutile TiO<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>by the screened-exchange hybrid functional. Physical Review B, 2012, 86, .	1.1	88
39	Structure of crystalline methanol at high pressure. Physical Review B, 1998, 58, R11809-R11812.	1.1	85
40	Electronic and magnetic properties of Ti₂O₃, Cr₂O₃, and Fe₂O₃calculated by the screened exchange hybrid density functional. Journal of Physics Condensed Matter, 2012, 24, 325504.	0.7	82
41	Comparison of the high-pressure and low-temperature structures of ethanol and acetic acid. Physical Review B, 1999, 60, 6328-6334.	1.1	79
42	High-pressure semiconductor-semimetal transition inTiS2. Physical Review B, 1998, 57, 5106-5110.	1.1	78
43	Hydrogen adsorption on the tetragonal ZrO2(101) surface: a theoretical study of an important catalytic reactantElectronic supplementary information (ESI) available: data for geometrical and charge differences in detail. See http://www.rsc.org/suppdata/cp/b2/b202330j/. Physical Chemistry Chemical Physics, 2002, 4, 3500-3508.	1.3	77
44	Concordant Epigenetic Silencing of Transforming Growth Factor-Î² Signaling Pathway Genes Occurs Early in Breast Carcinogenesis. Cancer Research, 2007, 67, 11517-11527.	0.4	76
45	Theoretical study of high-density phases of covalent semiconductors. I.Ab initiotreatment. Physical Review B, 1994, 49, 5329-5340.	1.1	74
46	The influence of pressure and temperature on the crystal structure of acetone. Chemical Communications, 1999, , 751-752.	2.2	70
47	Impeded Dimer Formation in the High-Pressure Crystal Structure of Formic Acid. Physical Review Letters, 1999, 82, 3464-3467.	2.9	67
48	Weed seed resources for birds in fields with contrasting conventional and genetically modified herbicide-tolerant crops. Proceedings of the Royal Society B: Biological Sciences, 2006, 273, 1921-1928.	1.2	61
49	Vibrational properties of the layered semiconductor germanium sulfide under hydrostatic pressure: Theory and experiment. Physical Review B, 1996, 53, 14806-14817.	1.1	59
50	Safety of vaccinations. Miss America, the media, and public health. JAMA - Journal of the American Medical Association, 1996, 276, 1869-1872.	3.8	59
51	Tetrahedral structures and phase transitions in III-V semiconductors. Physical Review B, 1994, 50, 8389-8401.	1.1	55
52	Parametrization and validation of a force field for liquid-crystal forming molecules. Physical Review E, 2002, 65, 051709.	0.8	55
53	Advances in understanding of transparent conducting oxides. Thin Solid Films, 2012, 520, 3714-3720.	0.8	53
54	Ab initiocalculations of the self-interstitial in silicon. Physical Review B, 1997, 56, 47-50.	1.1	51

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55	L-Cysteine-I at 30 K. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, o2739-o2742.	0.2	51
56	DFTâ€assisted interpretation of the Raman spectra of hydrogenâ€ordered ice XV. Journal of Raman Spectroscopy, 2013, 44, 290-298.	1.2	51
57	Conformation-dependent dipoles of liquid crystal molecules and fragments from first principles. Physical Review E, 1997, 55, 5641-5650.	0.8	48
58	Pressure-induced polymorphism in phenol. Acta Crystallographica Section B: Structural Science, 2002, 58, 1018-1024.	1.8	47
59	Pressure-Induced Polymerization of Polycyclic Areneâ€“Perfluoroarene Cocrystals: Single Crystal X-ray Diffraction Studies, Reaction Kinetics, and Design of Columnar Hydrofluorocarbons. Journal of the American Chemical Society, 2020, 142, 18907-18923.	6.6	47
60	Structural and electronic properties of L-amino acids. Physical Review B, 2005, 71, .	1.1	46
61	Defect energy states in high-K gate oxides. Physica Status Solidi (B): Basic Research, 2006, 243, 2071-2080.	0.7	45
62	Nonlocal density-functional description of exchange and correlation in silicon. Physical Review B, 2002, 65, .	1.1	44
63	Dielectric and vibrational properties of amino acids. Journal of Chemical Physics, 2004, 121, 5201-5210.	1.2	44
64	Condensed phase ionic polarizabilities from plane wave density functional theory calculations. Journal of Chemical Physics, 2006, 125, 144104.	1.2	42
65	Exotic structures of tetrahedral semiconductors. Reports on Progress in Physics, 1995, 58, 705-754.	8.1	41
66	High-pressure effects in the layered semiconductor germanium selenide. Physical Review B, 1995, 51, 16750-16760.	1.1	41
67	Calculation of the rotational viscosity of a nematic liquid crystal. Chemical Physics Letters, 2002, 356, 140-146.	1.2	41
68	Hexamer formation in tertiary butyl alcohol (2-methyl-2-propanol, C4H10O). Acta Crystallographica Section B: Structural Science, 2006, 62, 599-605.	1.8	39
69	Combining insights from solid-state NMR and first principles calculation: applications to the 19F NMR of octafluoronaphthalene. Physical Chemistry Chemical Physics, 2007, 9, 2389.	1.3	39
70	Density-functional calculations of semiconductor properties using a semiempirical exchange-correlation functional. Physical Review B, 2001, 63, .	1.1	38
71	Theoretical stability limit of diamond at ultrahigh pressure. Physical Review B, 1995, 52, 15035-15038.	1.1	37
72	Evidence for hydrogen transport in deuterated<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LiBH</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:ma low-temperature Raman-scattering measurements and first-principles calculations. Physical Review B, 2009, 80, .	K	37

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73	Compression mechanisms in quasimolecularXI3â€,(X=As,Sb,Bi)solids. Physical Review B, 1998, 58, 14812-14822.	1.1	36
74	Observation of magnetic excitons in LaCoO 3. Europhysics Letters, 2005, 70, 677-683.	0.7	36
75	An ab Initio Study of Observed and Hypothetical Polymorphs of Glycine. Crystal Growth and Design, 2005, 5, 1437-1442.	1.4	36
76	Theoretical study of high-density phases of covalent semiconductors. II. Empirical treatment. Physical Review B, 1994, 49, 5341-5352.	1.1	35
77	Matrix dependence of light emission from TCNQ adducts. Journal of Materials Chemistry, 2001, 11, 3053-3062.	6.7	35
78	First-principles studies of the structural and electronic properties of poly-para-phenylene vinylene. Journal of Physics Condensed Matter, 2004, 16, 8609-8620.	0.7	33
79	Calculation of flexoelectric coefficients for a nematic liquid crystal by atomistic simulation. Journal of Chemical Physics, 2004, 121, 9131-9139.	1.2	33
80	The Complex Excited-state Behavior of a Polyspirobifluorene Derivative: The Role of Spiroconjugation and Mixed Charge Transfer Character on Excited-state Stabilization and Radiative Lifetime. Journal of Physical Chemistry B, 2008, 112, 16300-16306.	1.2	33
81	Monomer Adsorption on Kaolinite: Modeling the Essential Ingredients. Journal of Physical Chemistry C, 2012, 116, 22365-22374.	1.5	33
82	[BDTA]2[Cu(mnt)2]:Â An Almost Perfect One-Dimensional Magnetic Material. Inorganic Chemistry, 2005, 44, 546-551.	1.9	32
83	Shifting Schottky barrier heights with ultra-thin dielectric layers. Microelectronic Engineering, 2011, 88, 1461-1463.	1.1	32
84	Using17O solid-state NMR and first principles calculation to characterise structure and dynamics in inorganic framework materials. Magnetic Resonance in Chemistry, 2007, 45, S144-S155.	1.1	31
85	Phase transitions in silicate perovskites from first principles. Mineralogical Magazine, 1998, 62, 585-598.	0.6	30
86	Role of Clay Minerals in Oil-Forming Reactions. Journal of Physical Chemistry A, 2010, 114, 3569-3575.	1.1	30
87	Terahertz time-domain spectroscopy of zone-folded acoustic phonons in 4H and 6H silicon carbide. Optics Express, 2019, 27, 3618.	1.7	29
88	First-principles calculations of2Ã—2reconstructions of GaN(0001) surfaces involving N, Al, Ga, In, and As atoms. Physical Review B, 2005, 72, .	1.1	28
89	Vibrational and elastic effects of point defects in silicon. Physical Review B, 1993, 48, 10899-10908.	1.1	27
90	Pressure-induced polymorphism in CuCl: Anab initiostudy. Physical Review B, 1995, 51, 12216-12222.	1.1	27

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91	Ab initioelasticity and lattice dynamics of. Journal of Physics Condensed Matter, 1997, 9, 375-380.	0.7	27
92	Electronic defects in LaAlO3. Microelectronic Engineering, 2008, 85, 65-69.	1.1	26
93	Calculation of semiconductor band structures and defects by the screened exchange density functional. Physica Status Solidi (B): Basic Research, 2011, 248, 537-546.	0.7	26
94	Stability and electronic structure of the cinnabar phase in GaAs. Physical Review B, 1998, 57, R2029-R2032.	1.1	25
95	The metalâ€“insulator phase change in vanadium dioxide and its applications. Journal of Applied Physics, 2021, 129, .	1.1	25
96	Ab initio molecular polarisabilities of liquid crystals: Application to DOBAMBC and 5CB. Europhysics Letters, 1998, 44, 578-584.	0.7	24
97	Field penetration induced charge redistribution effects on the field emission properties of carbon nanotubesâ€”a first-principle study. Applied Surface Science, 2004, 228, 143-150.	3.1	24
98	Gas molecule effects on field emission properties of single-walled carbon nanotube. Diamond and Related Materials, 2004, 13, 1306-1313.	1.8	24
99	Lattice dynamical and dielectric properties of L-amino acids. Physical Review B, 2006, 74, .	1.1	24
100	Structural Characterization and Physical Properties of the New Transition Metal Oxyselenide La₂O₂ZnSe₂. Inorganic Chemistry, 2013, 52, 2078-2085.	1.9	24
101	Calculation of metallic and insulating phases of V2O3 by hybrid density functionals. Journal of Chemical Physics, 2014, 140, 054702.	1.2	24
102	Properties of liquid crystal molecules from first principles computer simulation. Liquid Crystals, 1997, 22, 469-475.	0.9	23
103	On the identification of the oxygen vacancy in HfO2. Microelectronic Engineering, 2011, 88, 1464-1466.	1.1	23
104	A theoretical study of selenium I under high pressure. Journal of Physics Condensed Matter, 1993, 5, 8065-8074.	0.7	22
105	Conformational energy landscapes of liquid crystal molecules. Liquid Crystals, 1997, 22, 477-482.	0.9	22
106	Computation of magnetic shielding to simultaneously validate a crystal structure and assign a solid-state NMR spectrum. Journal of Molecular Structure, 2012, 1015, 192-201.	1.8	22
107	Super-radiant mode in InAsâ€”monolayerâ€“based Bragg structures. Scientific Reports, 2015, 5, 14911.	1.6	22
108	Comparison of bonding in amorphous silicon and carbon. Physical Review B, 1997, 55, 14059-14062.	1.1	21

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109	Valence-band offset of the lattice-matchedÎ²â^'FeSi2(100)/Si(001)heterostructure. Physical Review B, 2001, 63, .	1.1	21
110	Description of exchange and correlation in the strongly inhomogeneous electron gas using a nonlocal density functional. Physical Review B, 2002, 65, .	1.1	21
111	Ab initiocalculations of the structural and electronic properties ofHgmTenclusters. Physical Review B, 2004, 70, .	1.1	21
112	Origin of Magnetic Ordering in a Structurally Perfect Quantum Kagome Antiferromagnet. Physical Review Letters, 2020, 125, 027203.	2.9	21
113	Magnetic phases of antimonate-bearing <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>GaV</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:mrow><mml:mn>8</mml:mn><mml:mo>â^'</mml:mo><mml:mi>y</mml:mi></mml:mrow></mml:mrow></mml:math>		

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127	Interaction between Metallic p Orbitals and the Ï€ Orbitals of Organic Molecules:â€‰ The Binding between Ethylene and Aluminum. Journal of Physical Chemistry B, 2001, 105, 641-645.	1.2	14
128	A unique new multiband molecular conductor: [BDTA][Ni(dmit)2]2. Chemical Communications, 2005, , 3204.	2.2	14
129	Lattice dynamics of polyaniline and poly(p-pyridyl vinyline): First-principles determination. Physical Review B, 2006, 74, .	1.1	14
130	Iron reduction in nontronite-type clay minerals: Modelling a complex system. Geochimica Et Cosmochimica Acta, 2012, 81, 13-27.	1.6	14
131	Understanding Cationic Polymer Adsorption on Mineral Surfaces: Kaolinite in Cement Aggregates. Minerals (Basel, Switzerland), 2018, 8, 130.	0.8	14
132	Band Offset Models of Three-Dimensionally Bonded Semiconductors and Insulators. Journal of Physical Chemistry C, 2019, 123, 5562-5570.	1.5	14
133	Intrinsic Nature of Spontaneous Magnetic Fields in Superconductors with Time-Reversal Symmetry Breaking. Physical Review Letters, 2021, 127, 237002.	2.9	13
134	Transverse field muon-spin rotation measurement of the topological anomaly in a thin film of MnSi. Physical Review B, 2016, 93, .	1.1	12
135	A local Fock-exchange potential in Kohnâ€“Sham equations. Journal of Physics Condensed Matter, 2017, 29, 04LT01.	0.7	12
136	Quantum magnetism in molecular spin ladders probed with muon-spin spectroscopy. New Journal of Physics, 2018, 20, 103002.	1.2	12
137	Modelling the enthalpy change and transition temperature dependence of the metalâ€“insulator transition in pure and doped vanadium dioxide. Physical Chemistry Chemical Physics, 2020, 22, 13474-13478.	1.3	12
138	Comparison of the high-pressure and low-temperature structures of sulfuric acid. Dalton Transactions RSC, 2002, , 1867-1871.	2.3	11
139	Ab Initio Transition State Searching in Complex Systems: Fatty Acid Decarboxylation in Minerals.. Journal of Physical Chemistry A, 2011, 115, 2658-2667.	1.1	11
140	Theoretical adlayer surface morphology of wurtzite 2 Ã— 2 reconstructions of the GaN(0001) surface. Journal of Physics Condensed Matter, 2005, 17, 17-26.	0.7	10
141	The effects of screening length in the non-local screened-exchange functional. Journal of Physics Condensed Matter, 2015, 27, 025501.	0.7	10
142	Elucidation of the helical spin structure of FeAs. Physical Review B, 2017, 95, .	1.1	10
143	DFT+U investigation of the catalytic properties of ferruginous clay. American Mineralogist, 2013, 98, 132-140.	0.9	9
144	Muon-spin relaxation study of the double perovskite insulators Sr₂BOsO₆(Bâ€‰â€‰=â€‰â€‰Fe, Y, In). Journal of Physics Condensed Matter, 2016, 28, 076001.	0.7	9

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145	Hybrid band offset calculation for heterojunction interfaces between disparate semiconductors. Applied Physics Letters, 2020, 116, .	1.5	9
146	Megahertz dynamics in skyrmion systems probed with muon-spin relaxation. Physical Review B, 2021, 103, .	1.1	9
147	Magnetism and NÃ©el skyrmion dynamics in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>GaV</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:mo>⁢</mml:mo><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mrow><mml:mn>8</mml:mn><mml:mtext>âˆ’</mml:mtext><mml:mi>y</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math> Physical Review Research, 2020, 2, .	1.3	9
148	A theoretical study of pressure effects on selenium-I. Journal of Physics and Chemistry of Solids, 1995, 56, 329-334.	1.9	8
149	Breakdown of Rigid-Unit Vibrations in Layered Semiconductors under Pressure: Application to Germanium Sulfide. Europhysics Letters, 1995, 31, 151-155.	0.7	8
150	Exchange constants in molecule-based magnets derived from density functional methods. Physical Review B, 2017, 96, .	1.1	8
151	Local magnetism, magnetic order and spin freezing in the â€˜nonmetallic metalâ€™ FeCrAs. Journal of Physics Condensed Matter, 2019, 31, 285803.	0.7	8
152	Very low energy surface of silicon. Physical Review B, 1994, 50, 5728-5731.	1.1	7
153	Ab initiostudies of strained wurtzite GaN surfaces. Journal of Physics Condensed Matter, 2004, 16, 531-542.	0.7	7
154	Matrix dependence of blue light emission from a novel NH2-functionalized dicyanoquinodimethane derivative. Journal of Physical Organic Chemistry, 2006, 19, 206-213.	0.9	7
155	Extraordinarily Long-Ranged Structural Relaxation in Defective Achiral Carbon Nanotubes. Physical Review Letters, 2012, 109, 265502.	2.9	7
156	Determining the anisotropy and exchange parameters of polycrystalline spin-1 magnets. New Journal of Physics, 2019, 21, 093025.	1.2	7
157	Non-Local Density Functional Description of Poly- Para -Phenylene Vinylene. Chinese Physics Letters, 2007, 24, 807-810.	1.3	6
158	ELECTRONIC, MECHANICAL AND OPTICAL PROPERTIES OFSi₃P₄ANDGe₃P₄: ANAB INITIOSTUDY. International Journal of Modern Physics B, 2010, 24, 5487-5494.	1.3	6
159	Calculation of infrared and Raman vibration modes of magnesite at high pressure by density-functional perturbation theory and comparison with experiments. Physics and Chemistry of Minerals, 2011, 38, 193-202.	0.3	6
160	Calculation and interpretation of classical turning surfaces in solids. Npj Computational Materials, 2021, 7, .	3.5	6
161	Exchange-correlation holes in metal surfaces using nonlocal density-functional theory. Physical Review B, 2007, 76, .	1.1	5
162	Quantum mechanical tunneling in the automerization of cyclobutadiene. Journal of Chemical Physics, 2018, 148, 104109.	1.2	5

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163	Implications of bond disorder in a S=1 kagome lattice. Scientific Reports, 2018, 8, 4745.	1.6	5
164	Structural Refinement and Stability of Silicon XII. Materials Science Forum, 1996, 228-231, 595-600.	0.3	4
165	Investigation on exchange and correlation holes in a strongly confined electron gas. Journal of Physics Condensed Matter, 2004, 16, 4833-4844.	0.7	4
166	Self-interaction free local exchange potentials applied to metallic systems. Journal of Physics Condensed Matter, 2017, 29, 374002.	0.7	4
167	Energy-gap driven low-temperature magnetic and transport properties in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Cr</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>/</mml:mo><mml:mn>3</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mspace width="4pt" /><mml:mo>(</mml:mo><mml:mi>M</mml:mi></mml:mrow></mml:math>= Nb, Ta). Physical Review B, 2022, 105, .	1.1	4
168	Dense tetrahedral structures of compound semiconductors. Journal of Physics and Chemistry of Solids, 1995, 56, 495-500.	1.9	3
169	Transferability of first principles derived torsional potentials for mesogenic molecules and fragments. Molecular Physics, 1998, 93, 947-954.	0.8	3
170	Vibrational Properties of Liquid Crystal Molecules from AB Initio Computer Simulation. Molecular Crystals and Liquid Crystals, 1997, 302, 433-438.	0.3	2
171	Short-time reorientational processes in molecular fluids. Europhysics Letters, 2000, 49, 34-40.	0.7	2
172	A Quantitative Model for the Thermocouple Effect Using Statistical and Quantum Mechanics. AIP Conference Proceedings, 2003, , .	0.3	2
173	First-principles study of Oxygen deficiency in rutile Titanium Dioxide. Materials Research Society Symposia Proceedings, 2011, 1352, 3.	0.1	2
174	Magnetostructural relationship in the tetrahedral spin-chain oxideCsCoO2. Physical Review B, 2015, 91, .	1.1	2
175	Muon Tomography for Carbon Storage and Monitoring. Springer Proceedings in Physics, 2016, , 479-485.	0.1	2
176	Anomalous magnetic exchange in a dimerized quantum magnet composed of unlike spin species. Physical Review B, 2021, 104, .	1.1	2
177	The Effects of Government Expenditure on the Term Structure of Interest Rates: Comment. Journal of Money, Credit and Banking, 1985, 17, 397.	0.9	1
178	Ab initiomolecular dynamics of liquid carbon disulphide. Molecular Physics, 2001, 99, 855-863.	0.8	1
179	First-Principles Calculations of 2Ã—2 reconstructions of GaN Surfaces. AIP Conference Proceedings, 2005, , .	0.3	1
180	Screened Exchange Calculations of Semiconductor Band Structures. AIP Conference Proceedings, 2005, , .	0.3	1

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181	Molecular dynamics calculations of the thermal expansion properties and melting points of Si and Ge. Journal of Physics Condensed Matter, 2006, 18, 3489-3498.	0.7	1
182	Terahertz time-domain spectroscopy of crystalline and aqueous systems. , 2007, , .		1
183	Understanding the optical spectroscopy of amphiphilic molecular rectifiers: A density functional approach. Journal of Chemical Physics, 2010, 133, 244702.	1.2	1
184	The high-pressure electronic structure of the [Ni(ptdt)2] organic molecular conductor. Journal of Chemical Physics, 2012, 137, 024701.	1.2	1
185	Metastable structures of tetrahedral semiconductors. AIP Conference Proceedings, 1994, , .	0.3	0
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