

John S Tse

List of Publications by Year in descending order

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357
papers

16,262
citations

14655

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23533

111
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361
all docs

361
docs citations

361
times ranked

12525
citing authors

#	ARTICLE	IF	CITATIONS
1	Engineering the synergistic effect of carbon dots-stabilized atomic and subnanometric ruthenium as highly efficient electrocatalysts for robust hydrogen evolution. <i>SmartMat</i> , 2022, 3, 249-259.	10.7	38
2	Desmarais <i>et al.</i> Reply. <i>Physical Review Letters</i> , 2022, 128, 099702.	7.8	0
3	Theory-directed discovery of high-temperature superconductivity in clathrate hydrides at high pressure. <i>Innovation(China)</i> , 2022, 3, 100226.	9.1	4
4	Lithiation MAX derivative electrodes with low overpotential and long-term cyclability in a wide-temperature range. <i>Energy Storage Materials</i> , 2022, 47, 611-619.	18.0	3
5	Carbonate melts under lower mantle conditions. <i>Science Bulletin</i> , 2022, , .	9.0	1
6	Turning on Zn 4s Electrons in a $N_{2\rightarrow}Zn_{2\rightarrow}$ Configuration to Stimulate Remarkable ORR Performance. <i>Angewandte Chemie</i> , 2021, 133, 183-187.	2.0	42
7	Turning on Zn 4s Electrons in a $N_{2\rightarrow}Zn_{2\rightarrow}$ Configuration to Stimulate Remarkable ORR Performance. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 181-185.	13.8	161
8	New-phase retention in colloidal core/shell nanocrystals <i>via</i> pressure-modulated phase engineering. <i>Chemical Science</i> , 2021, 12, 6580-6587.	7.4	6
9	Single Atom Ruthenium-Doped CoP/CDs Nanosheets via Splicing of Carbon Dots for Robust Hydrogen Production. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 7234-7244.	13.8	306
10	Single Atom Ruthenium-Doped CoP/CDs Nanosheets via Splicing of Carbon Dots for Robust Hydrogen Production. <i>Angewandte Chemie</i> , 2021, 133, 7310-7320.	2.0	13
11	Chemical physics of superconductivity in layered yttrium carbide halides from first principles. <i>Physical Review B</i> , 2021, 103, .	3.2	0
12	Mechanisms for Pressure-Induced Isostructural Phase Transitions in EuO. <i>Physical Review Letters</i> , 2021, 126, 196404.	7.8	7
13	^{57}Fe Mössbauer isomer shift of pure iron and iron oxides at high pressure—An experimental and theoretical study. <i>Journal of Chemical Physics</i> , 2021, 154, 214104.	3.0	4
14	High-Pressure Nonequilibrium Dynamics on Second-to-Microsecond Time Scales: Application of Time-Resolved X-ray Diffraction and Dynamic Compression in Ice. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 8024-8038.	4.6	5
15	In situ X-ray diffraction study of chrysotile at high P - T conditions: transformation to the 3.65 Å... phase. <i>Physics and Chemistry of Minerals</i> , 2021, 48, 1.	0.8	0
16	A comparative study on pressure-induced structural transformations in a basaltic glass and melt from Ab initio molecular dynamics calculations. <i>Physics and Chemistry of Minerals</i> , 2021, 48, 1.	0.8	3
17	In Situ X-Ray Diffraction Study on Hydrate Formation at Low Temperature in a High Vacuum. <i>Journal of Physical Chemistry C</i> , 2021, 125, 26892-26900.	3.1	5
18	Onset of anharmonicity and thermal conductivity in SnSe. <i>Physical Review B</i> , 2021, 104, .	3.2	5

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19	A chemical perspective on high pressure crystal structures and properties. National Science Review, 2020, 7, 149-169.	9.5	25
20	High-Density COH_x Network Glass. Journal of Physical Chemistry C, 2020, 124, 107-114.	3.1	3
21	Temperature- and Rate-Dependent Pathways in Formation of Metastable Silicon Phases under Rapid Decompression. Physical Review Letters, 2020, 125, 155702.	7.8	18
22	Structural dynamics of basaltic melt at mantle conditions with implications for magma oceans and superplumes. Nature Communications, 2020, 11, 4815.	12.8	17
23	Slow compression of crystalline ice at low temperature. Nature, 2020, 585, E9-E10.	27.8	4
24	Thermal Conductivity of High-Temperature Phases of Cu ₂ S from Ab Initio Molecular Dynamics: Advent of Lattice-Site Hopping. Journal of Physical Chemistry C, 2020, 124, 12318-12323.	3.1	0
25	Compression behavior of dense H_2 mixtures up to 160 GPa. Physical Review B, 2020, 101, .	3.2	5
26	Temperature-dependent kinetic pathways featuring distinctive thermal-activation mechanisms in structural evolution of ice VII. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 15437-15442.	7.1	9
27	Synthesis of Atomically Thin Hexagonal Diamond with Compression. Nano Letters, 2020, 20, 5916-5921.	9.1	42
28	An automated predictor for identifying transition states in solids. Npj Computational Materials, 2020, 6, .	8.7	12
29	Possibility of realizing superionic ice VII in external electric fields of planetary bodies. Science Advances, 2020, 6, eaaz2915.	10.3	18
30	Classical and path-integral molecular-dynamics study on liquid water and ice melting using non-empirical TTM2.1-F model. Molecular Physics, 2019, 117, 3241-3253.	1.7	1
31	X-Ray Diffraction Study of Chrysotile Compressed in Water under High P&T Conditions of up to 8 GPa and 420Å ³ . Bulletin of the Russian Academy of Sciences: Physics, 2019, 83, 687-690.	0.6	1
32	A twist in the tale of the structure of ice. Nature, 2019, 569, 495-496.	27.8	5
33	Large bandgap of pressurized trilayer graphene. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 9186-9190.	7.1	59
34	Hard BN Clathrate Superconductors. Journal of Physical Chemistry Letters, 2019, 10, 2554-2560.	4.6	14
35	Mechanism for the Structural Transformation to the Modulated Superconducting Phase of Compressed Hydrogen Sulfide. Scientific Reports, 2019, 9, 5023.	3.3	12
36	First-Principles Methods in the Investigation of the Chemical and Transport Properties of Materials under Extreme Conditions. Engineering, 2019, 5, 421-433.	6.7	4

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37	Pancakes under Pressure: A Case Study on Isostructural Dithia- and Diselenadiazolyl Radical Dimers. <i>Inorganic Chemistry</i> , 2019, 58, 3550-3557.	4.0	7
38	Itinerant ferromagnetic half metallic cobalt-iron couples: promising bifunctional electrocatalysts for ORR and OER. <i>Journal of Materials Chemistry A</i> , 2019, 7, 27175-27185.	10.3	122
39	Benzoquinone-Bridged Heterocyclic Zwitterions as Building Blocks for Molecular Semiconductors and Metals. <i>Inorganic Chemistry</i> , 2018, 57, 4757-4770.	4.0	20
40	Frontispiece: Superconducting Hydrogen Sulfide. <i>Chemistry - A European Journal</i> , 2018, 24, .	3.3	0
41	Crystal Structures and Electronic Properties of Xe-Cl Compounds at High Pressure. <i>Journal of Physical Chemistry C</i> , 2018, 122, 2941-2950.	3.1	7
42	Polymer-Passivated Inorganic Cesium Lead Mixed-Halide Perovskites for Stable and Efficient Solar Cells with High Open-Circuit Voltage over 1.3 V. <i>Advanced Materials</i> , 2018, 30, 1705393.	21.0	401
43	Thermal Conductivity of Solids from First-Principles Molecular Dynamics Calculations. <i>Journal of Physical Chemistry C</i> , 2018, 122, 10682-10690.	3.1	16
44	Mechanism of Chemical Reactions between SiO ₂ and CO ₂ under Mantle Conditions. <i>ACS Earth and Space Chemistry</i> , 2018, 2, 548-555.	2.7	12
45	Uptake and speciation of uranium in synthetic gypsum (CaSO ₄ · 2H ₂ O): Applications to radioactive mine tailings. <i>Journal of Environmental Radioactivity</i> , 2018, 181, 8-17.	1.7	22
46	Structures and Transport Properties of CaCO ₃ Melts under Earth's Mantle Conditions. <i>ACS Earth and Space Chemistry</i> , 2018, 2, 1-8.	2.7	15
47	Superconducting Hydrogen Sulfide. <i>Chemistry - A European Journal</i> , 2018, 24, 1769-1778.	3.3	32
48	Venture into Water's No Man's Land: Structural Transformations of Solid H_2O under Rapid Compression and Decompre	7.8	21
49	Dynamics and superconductivity in compressed lanthanum superhydride. <i>Physical Review B</i> , 2018, 98, .	3.2	85
50	Structures and Stability of Iron Halides at the Earth's Mantle and Core Pressures: Implications for the Missing Halogen Paradox. <i>ACS Earth and Space Chemistry</i> , 2018, 2, 711-719.	2.7	8
51	Spin localization, magnetic ordering, and electronic properties of strongly correlated Ln_2O_3 sesquioxides (Ln=La, Ce, Pr, Nd). <i>Physical Review B</i> , 2018, 97, .	3.2	36
52	Carbon-Quantum-Dots-Loaded Ruthenium Nanoparticles as an Efficient Electrocatalyst for Hydrogen Production in Alkaline Media. <i>Advanced Materials</i> , 2018, 30, e1800676.	21.0	406
53	Reply to Datchi et al.: Recovered phase CO ₂ -V at low temperature and a newly predicted 3D-extended CO ₂ phase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E658-E659.	7.1	1
54	The Power of Packing: Metallization of an Organic Semiconductor. <i>Journal of the American Chemical Society</i> , 2017, 139, 2180-2183.	13.7	48

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55	Formation and properties of water from quartz and hydrogen at high pressure and temperature. Earth and Planetary Science Letters, 2017, 461, 54-60.	4.4	13
56	Fine Tuning the Performance of Multiorbital Radical Conductors by Substituent Effects. Journal of the American Chemical Society, 2017, 139, 1625-1635.	13.7	40
57	Hydrogen-Doped Polymeric Carbon Monoxide at High Pressure. Journal of Physical Chemistry C, 2017, 121, 10078-10086.	3.1	11
58	Crystal Structures of CaB ₃ N ₃ at High Pressures. Inorganic Chemistry, 2017, 56, 7449-7453.	4.0	2
59	Piezochromic Carbon Dots with Two-photon Fluorescence. Angewandte Chemie - International Edition, 2017, 56, 6187-6191.	13.8	223
60	Solid-State Polymerization of CO ₂ from Catalytic Photoexcitation: An Ab Initio Molecular Dynamics Study. Journal of Physical Chemistry C, 2017, 121, 115-122.	3.1	2
61	Kinetically Controlled Two-Step Amorphization and Amorphous-Amorphous Transition in Ice. Physical Review Letters, 2017, 119, 135701.	7.8	22
62	Electron-phonon coupling mechanisms for hydrogen-rich metals at high pressure. Physical Review B, 2017, 96, .	3.2	56
63	Modulated Structure Calculated for Superconducting Hydrogen Sulfide. Angewandte Chemie, 2017, 129, 11548-11551.	2.0	4
64	Modulated Structure Calculated for Superconducting Hydrogen Sulfide. Angewandte Chemie - International Edition, 2017, 56, 11390-11393.	13.8	21
65	optPBE-vdW density functional theory study of liquid water and pressure-induced structural evolution in ice Ih. Canadian Journal of Chemistry, 2017, 95, 1205-1211.	1.1	6
66	Melting and High Pressure Transitions of Hydrogen up to 300 GPa. Physical Review Letters, 2017, 119, 075302.	13.8	139
67	Superconductivity in FeH ₅ . Physical Review B, 2017, 96, .	3.2	145
68	Equilibrium Born-Oppenheimer molecular-dynamics exploration of the lattice thermal conductivity of silicon clathrates. Computational Materials Science, 2017, 126, 1-6.	3.0	9
69	Oxygen Packing Fraction and the Structure of Silicon and Germanium Oxide Glasses. Journal of Physical Chemistry B, 2017, 121, 10726-10732.	2.6	23
70	Predicted lithium-iron compounds under high pressure. RSC Advances, 2016, 6, 66721-66728.	3.6	4
71	Prediction of Host-Guest Na-Fe Intermetallics at High Pressures. Inorganic Chemistry, 2016, 55, 7026-7032.	4.0	8
72	Low-density superhard materials: computational study of Li-inserted B-substituted closo-carboranes LiB ₁₁ and Li ₂ B ₂ C ₁₀ . RSC Advances, 2016, 6, 52695-52699.	3.6	8

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73	A New Allotrope of Nitrogen as High-Energy Density Material. <i>Journal of Physical Chemistry A</i> , 2016, 120, 2920-2925.	2.5	73
74	Pressure-induced polyamorphism in a main-group metallic glass. <i>Physical Review B</i> , 2016, 94, .	3.2	14
75	Electronic structures of greigite (Fe ₃ S ₄): A hybrid functional study and prediction for a Verwey transition. <i>Scientific Reports</i> , 2016, 6, 21637.	3.3	11
76	Crystal structures and dynamical properties of dense CO ₂ . <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 11110-11115.	7.1	28
77	Superconductivity in dense carbon-based materials. <i>Physical Review B</i> , 2016, 93, .	3.2	37
78	Unusual Li-Ion Transfer Mechanism in Liquid Electrolytes: A First-Principles Study. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4795-4801.	4.6	39
79	Pushing T _C to 27.5 K in a heavy atom radical ferromagnet. <i>Chemical Communications</i> , 2016, 52, 13877-13880.	4.1	21
80	Anomalous bond length behavior and a new solid phase of bromine under pressure. <i>Scientific Reports</i> , 2016, 6, 25649.	3.3	13
81	New Raman measurements for H ₂ O ice VII in the range of 300 cm ⁻¹ to 4000 cm ⁻¹ at pressures up to 120 GPa. <i>Journal of Chemical Physics</i> , 2016, 145, 124315.	3.0	20
82	Tunable Excitonic Processes at Organic Heterojunctions. <i>Advanced Materials</i> , 2016, 28, 649-654.	21.0	38
83	pH-Dependent Synthesis of Novel Structure-Controllable Polymer-Carbon NanoDots with High Acidophilic Luminescence and Super Carbon Dots Assembly for White Light-Emitting Diodes. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 4062-4068.	8.0	106
84	Crystal Structure and Superconductivity of PH ₃ at High Pressures. <i>Journal of Physical Chemistry C</i> , 2016, 120, 3458-3461.	3.1	78
85	Bulk sensitive determination of the Fe ³⁺ /Fe ^{Tot} -ratio in minerals by Fe L _{2/3} -edge X-ray Raman scattering. <i>Journal of Analytical Atomic Spectrometry</i> , 2016, 31, 815-820.	3.0	9
86	Massively parallel molecular dynamics simulation of formation of ice-crystallite precursors in supercooled water: Incipient-nucleation behavior and role of system size. <i>Physical Review E</i> , 2015, 92, 032132.	2.1	13
87	High-Energy Density and Superhard Nitrogen-Rich B-N Compounds. <i>Physical Review Letters</i> , 2015, 115, 105502.	7.8	132
88	The electrical conductivity of Al ₂ O ₃ under shock-compression. <i>Scientific Reports</i> , 2015, 5, 12823.	3.3	8
89	Pressure-induced phase transition and electrical properties of thermoelectric Al-doped Mg ₂ Si. <i>Journal of Applied Physics</i> , 2015, 118, .	2.5	12
90	Stability and properties of liquid CO ₂ at high pressure and high temperature: Implications for electrical conductivities in Earth's lower mantle. <i>Geophysical Research Letters</i> , 2015, 42, 5820-5827.	4.0	3

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91	High pressure–low temperature phase diagram of barium: Simplicity versus complexity. Applied Physics Letters, 2015, 107, .	3.3	9
92	Mechanisms for pressure-induced crystal-crystal transition, amorphization, and devitrification of SnI ₄ . Journal of Chemical Physics, 2015, 143, 164508.	3.0	13
93	Rietveld refinement using synchrotron powder diffraction data for curcumin, C ₂₁ H ₂₀ O ₆ , and comparison with density functional theory. Powder Diffraction, 2015, 30, 67-75.	0.2	10
94	Prediction of novel crystal structures and superconductivity of compressed HBr. RSC Advances, 2015, 5, 45812-45816.	3.6	6
95	Pressure-stabilized superconductive yttrium hydrides. Scientific Reports, 2015, 5, 9948.	3.3	257
96	Structures of the metallic and superconducting high pressure phases of solid CS ₂ . Scientific Reports, 2015, 5, 10458.	3.3	18
97	Modification of surface chemistry by lattice Sn doping in BiFeO ₃ nanofibers. Europhysics Letters, 2015, 111, 18005.	2.0	9
98	Enhanced figure of merit in Mg ₂ Si _{0.877} Ge _{0.1} Bi _{0.023} /multi wall carbon nanotube nanocomposites. RSC Advances, 2015, 5, 65328-65336.	3.6	20
99	Origin of pressure-induced crystallization of Ce ₇₅ Al ₂₅ metallic glass. Nature Communications, 2015, 6, 6493.	12.8	33
100	Crystal Structures and Chemical Bonding of Magnesium Carbide at High Pressure. Journal of Physical Chemistry C, 2015, 119, 23168-23174.	3.1	18
101	The Metallic State in Neutral Radical Conductors: Dimensionality, Pressure and Multiple Orbital Effects. Journal of the American Chemical Society, 2015, 137, 14136-14148.	13.7	37
102	Mixing unmixables: Unexpected formation of Li-Cs alloys at low pressure. Science Advances, 2015, 1, e1500669.	10.3	16
103	Thermoelectric and electrical transport properties of Mg ₂ Si multi-doped with Sb, Al and Zn. Journal of Materials Chemistry A, 2015, 3, 19774-19782.	10.3	39
104	Pressure induced spin transition revealed by iron M _{2,3} -edge spectroscopy. Applied Physics Letters, 2014, 104, .	3.3	18
105	Dihydrogen Bonding in Compressed Ammonia Borane and Its Roles in Structural Stability. Journal of Physical Chemistry C, 2014, 118, 29591-29598.	3.1	24
106	Comment on "State-Dependent Electron Delocalization Dynamics at the Solute-Solvent Interface: Soft-X-Ray Absorption Spectroscopy and Ab Initio Calculations". Physical Review Letters, 2014, 112, 129301.	7.8	11
107	Speciation and distribution of copper in a mining soil using multiple synchrotron-based bulk and microscopic techniques. Environmental Science and Pollution Research, 2014, 21, 2943-2954.	5.3	44
108	Iron speciation in minerals and glasses probed by M _{2/3} -edge X-ray Raman scattering spectroscopy. Contributions To Mineralogy and Petrology, 2014, 167, 1.	3.1	18

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109	Robust Diffusive Proton Motions in Phase IV of Solid Hydrogen. <i>Journal of Physical Chemistry C</i> , 2014, 118, 11902-11905.	3.1	7
110	Pressure-Induced Changes on The Electronic Structure and Electron Topology in the Direct FCC \rightarrow SH Transformation of Silicon. <i>Journal of Physical Chemistry C</i> , 2014, 118, 1161-1166.	3.1	20
111	Thermal Conductivity of Supercooled Water: An Equilibrium Molecular Dynamics Exploration. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 3819-3824.	4.6	15
112	Reversible pressure-induced crystal-amorphous structural transformation in ice Ih. <i>Chemical Physics Letters</i> , 2014, 609, 54-58.	2.6	9
113	Electronic and magnetic structure of neutral radical FBBO. <i>Physical Review B</i> , 2014, 89, .	3.2	17
114	Pressure Induced Phase Transitions and Metallization of a Neutral Radical Conductor. <i>Journal of the American Chemical Society</i> , 2014, 136, 1070-1081.	13.7	72
115	Heat, Pressure and Light-Induced Interconversion of Bisdithiazolyl Radicals and Dimers. <i>Journal of the American Chemical Society</i> , 2014, 136, 8050-8062.	13.7	63
116	Bonding, structures, and band gap closure of hydrogen at high pressures. <i>Physical Review B</i> , 2013, 87, .	3.2	54
117	<i>Allium fistulosum</i> as a novel system to investigate mechanisms of freezing resistance. <i>Physiologia Plantarum</i> , 2013, 147, 101-111.	5.2	23
118	Silicon clathrates as anode materials for lithium ion batteries?. <i>Journal of Materials Chemistry A</i> , 2013, 1, 7782.	10.3	42
119	Electronic structure of carbon dioxide under pressure and insights into the molecular-to-nonmolecular transition. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 18402-18406.	7.1	24
120	Indentation strength of ultraincompressible rhenium boride, carbide, and nitride from first-principles calculations. <i>Physical Review B</i> , 2012, 86, .	3.2	58
121	Pressure-induced amorphization of methane hydrate. <i>Physical Review B</i> , 2012, 86, .	3.2	15
122	Electron band structure of the high pressure cubic phase of AlH_3 . <i>Journal of Physics: Conference Series</i> , 2012, 377, 012093.	0.4	7
123	Structure and Properties of Dense Silica Glass. <i>Scientific Reports</i> , 2012, 2, 398.	3.3	80
124	Pressure amorphized ices – an atomistic perspective. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 8255.	2.8	20
125	Dark channel fluorescence observations result from concentration effects rather than solvent-solute charge transfer. <i>Nature Chemistry</i> , 2012, 4, 765-766.	13.6	22
126	Polymerization of Carbon Dioxide: A Chemistry View of Molecular-to-Nonmolecular Phase Transitions. <i>Journal of Physical Chemistry C</i> , 2012, 116, 2061-2067.	3.1	19

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127	Superconductive sodalite-like clathrate calcium hydride at high pressures. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 6463-6466.	7.1	630
128	A Pressure Induced Structural Dichotomy in Isostructural Bis-1,2,3-thiaselenazolyl Radical Dimers. Crystal Growth and Design, 2012, 12, 4676-4684.	3.0	15
129	Crossing the Insulator-to-Metal Barrier with a Thiazyl Radical Conductor. Journal of the American Chemical Society, 2012, 134, 9886-9889.	13.7	75
130	First-Principles Study on the Mechanisms for H ₂ Formation in Ammonia Borane at Ambient and High Pressure. Journal of Physical Chemistry C, 2012, 116, 2146-2152.	3.1	19
131	Li Ion Diffusion Mechanisms in LiFePO ₄ : An ab Initio Molecular Dynamics Study. Journal of Physical Chemistry A, 2011, 115, 13045-13049.	2.5	107
132	Dynamical Properties of Hydrogen Sulphide Motion in its Clathrate Hydrate from Ab Initio and Classical Isobaric Isothermal Molecular Dynamics. Journal of Physical Chemistry A, 2011, 115, 6226-6232.	2.5	24
133	From Magnets to Metals: The Response of Tetragonal Bisdiselenazolyl Radicals to Pressure. Journal of the American Chemical Society, 2011, 133, 6051-6060.	13.7	89
134	Soft X-ray Induced Photoreduction of Organic Cu(II) Compounds Probed by X-ray Absorption Near-Edge (XANES) Spectroscopy. Analytical Chemistry, 2011, 83, 7856-7862.	6.5	38
135	Insulator-metal transition of highly compressed carbon disulfide. Physical Review B, 2011, 84, .	3.2	20
136	Magnetic behavior of Fe(Se,Te) systems: First-principles calculations. Journal of Applied Physics, 2011, 110, .	2.5	23
137	Pressure-induced electron topological transitions in Ba-doped Si clathrate. Physical Review B, 2011, 84, .	3.2	17
138	Thermal conduction and phonon propagation in pressure-amorphized ices. Physical Review B, 2011, 83, .	3.2	12
139	Phonon density of states of Fe ₂ O ₃ across high-pressure structural and electronic transitions. Physical Review B, 2011, 84, .	3.2	12
140	Dynamics of Kr in dense clathrate hydrates. Physical Review B, 2011, 83, .	3.2	8
141	ELECTRONIC AND MAGNETIC STRUCTURE OF THE HIGH PRESSURE PHASE OF Li ₂ CuO ₂ . International Journal of Modern Physics B, 2011, 25, 3409-3414.	2.0	4
142	Intrinsic hardness of crystalline solids. Journal of Superhard Materials, 2010, 32, 177-191.	1.2	63
143	Bonding in the ϵ -Type Ferropnictide Superconductor LiFeAs. Journal of Superconductivity and Novel Magnetism, 2010, 23, 579-581.	1.8	0
144	Origin of anisotropy and metallic behavior in delafossite PdCoO ₂ . Physical Review B, 2010, 81, .	3.2	49

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145	Perspectives on Hydrate Thermal Conductivity. <i>Energies</i> , 2010, 3, 1934-1942.	3.1	26
146	Unzipping of Graphene by Fluorination. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 1394-1397.	4.6	16
147	Metallization of a Hypervalent Radical Dimer: Molecular and Band Perspectives. <i>Journal of the American Chemical Society</i> , 2010, 132, 4876-4886.	13.7	39
148	Hysteretic Spin Crossover between a Bisdithiazolyl Radical and Its Hypervalent σ -Dimer. <i>Journal of the American Chemical Society</i> , 2010, 132, 16212-16224.	13.7	102
149	Thermal conductivity in amorphous ices from molecular dynamics. <i>Physical Review B</i> , 2010, 82, .	3.2	22
150	Superconducting high-pressure phase of cesium iodide. <i>Physical Review B</i> , 2009, 79, .	3.2	27
151	Mechanisms for thermal conduction in various polymorphs of methane hydrate. <i>Physical Review B</i> , 2009, 80, .	3.2	61
152	Lattice distortion of hcp solid helium under pressure. <i>Physical Review B</i> , 2009, 80, .	3.2	22
153	Toward a comprehensive understanding of solid-state core-level XPS linewidths: Experimental and theoretical studies on the Si^{2p} core level. <i>Physical Review B</i> , 2009, 80, .	3.2	63
154	Core effects on the energetics of solid Li at high pressure. <i>Physical Review B</i> , 2009, 79, .	3.2	5
155	Crystal and electronic structure of superhard BC_2S . First-principles structural optimizations. <i>Physical Review B</i> , 2009, 80, .	3.2	39
156	Superconductivity in lithium under high pressure investigated with density functional and Eliashberg theory. <i>Physical Review B</i> , 2009, 79, .	3.2	48
157	A comparative study on the LDA + U and hybrid functional methods on the description of the electronic structure of YTiO_3 under high pressure. <i>Canadian Journal of Chemistry</i> , 2009, 87, 1374-1382.	1.1	3
158	Comment on "New Metallic Carbon Crystal". <i>Physical Review Letters</i> , 2009, 102, 229601.	7.8	55
159	Instability of CaLi_2 at high pressure: Theoretical prediction and experimental results. <i>Europhysics Letters</i> , 2009, 86, 56001.	2.0	13
160	Boron charged under pressure. <i>Nature</i> , 2009, 457, 800-801.	27.8	13
161	High-pressure structures and vibrational spectra of barium fluoride: Results obtained under nearly hydrostatic conditions. <i>Physical Review B</i> , 2009, 79, .	3.2	13
162	Effect of pressure on the iron arsenide superconductor LiFeAs .		

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163	Heavy Atom Ferromagnets under Pressure: Structural Changes and the Magnetic Response. Journal of the American Chemical Society, 2009, 131, 16012-16013.	13.7	60
164	Crystal, spin, and electronic structure of the superconductor LiFeAs. Physical Review B, 2009, 80, .	3.2	21
165	Isostructural Bis-1,2,3-Thiaselenazolyl Dimers. Inorganic Chemistry, 2009, 48, 9874-9882.	4.0	30
166	Mechanisms for Thermal Conduction in Methane Hydrate. Physical Review Letters, 2009, 103, 015901.	7.8	78
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