

# First principles methods using CASTEP

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Variational density-functional perturbation theory for dielectrics and lattice dynamics. <i>Physical Review B</i> , 2006, 73, .	1.1	735
2	Spectroscopic and Ab Initio Characterization of the [ReH <sub>9</sub> ] <sup>2-</sup> Ion. <i>Inorganic Chemistry</i> , 2006, 45, 10951-10957.	1.9	25
3	Screened-exchange stress tensor in density functional theory. <i>Physical Review B</i> , 2006, 73, .	1.1	15
4	Density Functional Theory Based Ab Initio Molecular Dynamics Using the Car-Parrinello Approach. , 2006, , 223-285.		9
5	Implementation of linear-scaling plane wave density functional theory on parallel computers. <i>Physica Status Solidi (B): Basic Research</i> , 2006, 243, 973-988.	0.7	44
6	Lattice dynamical and dielectric properties of L-amino acids. <i>Physical Review B</i> , 2006, 74, .	1.1	24
7	When is H <sub>2</sub> O not water?. <i>Journal of Chemical Physics</i> , 2007, 127, 244503.	1.2	28
8	Achieving plane wave accuracy in linear-scaling density functional theory applied to periodic systems: A case study on crystalline silicon. <i>Journal of Chemical Physics</i> , 2007, 127, 164712.	1.2	46
9	Graphite intercalation compounds under pressure: A first-principles density functional theory study. <i>Physical Review B</i> , 2007, 75, .	1.1	35
10	A density functional study of the effect of hydrogen on the strength of an epitaxial Ag/ZnO interface. <i>Journal of Applied Physics</i> , 2007, 102, 103513.	1.1	12
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12	Coupled Al/Si and O/N order/disorder in BaYb[Si <sub>4</sub> Al <sub>x</sub> O <sub>7</sub> ] <sub>2</sub> silon: neutron powder diffraction and Monte Carlo simulations. <i>Zeitschrift für Kristallographie</i> , 2007, 222, .	1.1	11
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14	NMR crystallography of oxybuprocaine hydrochloride, Modification II <sup>o</sup> . <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 360-368.	1.3	102
15	Density functional theory study of flat and stepped NaCl(001). <i>Physical Review B</i> , 2007, 76, .	1.1	40
16	WO <sub>3</sub> Nanorods Synthesized on a Thermal Hot Plate. <i>Journal of Physical Chemistry C</i> , 2007, 111, 17193-17199.	1.5	32
17	Carbon-13 Chemical Shift Tensors of Disaccharides: A Measurement, Computation and Assignment. <i>Journal of Physical Chemistry A</i> , 2007, 111, 13126-13132.	1.1	44
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3593	Enhanced magnetoelectric effect in M-type hexaferrites by Co substitution into trigonal bi-pyramidal sites. <i>Applied Physics Letters</i> , 2018, 112, 082401.	1.5	20
3594	Effect of Element Substitution on Structural Transformation and Optical Performances in $\text{BaM}_{\text{IV}}\text{Q}_4$ ( $\text{M}_{\text{IV}} = \text{Li, Na, Cu, and Ag}$ ; $\text{M}_{\text{IV}} = \text{Tj, ET, Q, Rh}$ )	1.0	78
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3715	Band edge states, intrinsic defects, and dopants in monolayer HfS <sub>2</sub> and SnS <sub>2</sub> . <i>Applied Physics Letters</i> , 2018, 112, .	1.5	22
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4073	A Bifunctional MOF Catalyst Containing Metal-Phosphine and Lewis Acidic Active Sites. <i>Chemistry - A European Journal</i> , 2018, 24, 15309-15318.	1.7	40
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4087	A stable <i>C<sub>2</sub>m</i> phase of H <sub>2</sub> S at 150-175 GPa. <i>Japanese Journal of Applied Physics</i> , 2018, 57, 083101.	0.8	1
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4098	Density functional theory study of Al/NbB <sub>2</sub> heterogeneous nucleation interface. <i>Applied Surface Science</i> , 2018, 456, 37-42.	3.1	39
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4104	Structural, elastic, mechanical and thermodynamic properties of HfB <sub>4</sub> under high pressure. <i>Royal Society Open Science</i> , 2018, 5, 180701.	1.1	10
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4106	Successful Computationally Directed Templating of Metastable Pharmaceutical Polymorphs. <i>Crystal Growth and Design</i> , 2018, 18, 5322-5331.	1.4	52
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4109	Atomic-level insight into super-efficient electrocatalytic oxygen evolution on iron and vanadium co-doped nickel (oxy)hydroxide. <i>Nature Communications</i> , 2018, 9, 2885.	5.8	669
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4113	Module-Guided Design Scheme for Deep-Ultraviolet Nonlinear Optical Materials. <i>Journal of the American Chemical Society</i> , 2018, 140, 10726-10733.	6.6	127
4114	Hierarchical tandem assembly of planar [3Å–3] building units into {3Å–[3Å–3]} oligomers: mixed-valency, electrical conductivity and magnetism. <i>Chemical Science</i> , 2018, 9, 7498-7504.	3.7	23
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4118	Electronic and mechanical properties of C/Si phases with sp <sup>2</sup> and sp <sup>3</sup> hybridization: A first-principles study. <i>AIP Advances</i> , 2018, 8, 075326.	0.6	0
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4120	First-principles hydrogen adsorption properties of Li-decorated ThMoB <sub>4</sub> -type graphene. <i>International Journal of Hydrogen Energy</i> , 2018, 43, 16117-16127.	3.8	10
4121	Scale-Up Biomass Pathway to Cobalt Single-Site Catalysts Anchored on N-Doped Porous Carbon Nanobelt with Ultrahigh Surface Area. <i>Advanced Functional Materials</i> , 2018, 28, 1802167.	7.8	112
4122	Roads to pentazolate anion: a theoretical insight. <i>Royal Society Open Science</i> , 2018, 5, 172269.	1.1	10
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4125	Becquerelite mineral phase: crystal structure and thermodynamic and mechanical stability by using periodic DFT. <i>RSC Advances</i> , 2018, 8, 24599-24616.	1.7	36

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4138	Charged Si <sub>9</sub> Clusters in Neat Solids and the Detection of [H <sub>2</sub> Si <sub>9</sub> ] <sup>2+</sup> in Solution: A Combined NMR, Raman, Mass Spectrometric, and Quantum Chemical Investigation. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 12950-12955.	7.2	28
4139	Interfacial stability, electronic property, and surface reactivity of $\hat{\pm}$ -MoO <sub>3</sub> / $\hat{\pm}$ -Al <sub>2</sub> O <sub>3</sub> composites: DFT and DFT+ $\hat{\epsilon}$ calculations. <i>Computational Materials Science</i> , 2018, 153, 217-227.	1.4	8
4140	Two noncentrosymmetric polyphosphates featuring infinite one-dimensional (PO <sub>3</sub> ) <sup>-</sup> chain, LiMP <sub>2</sub> O <sub>6</sub> (M = Rb, Cs): Synthesis, structure and optical properties. <i>Journal of Solid State Chemistry</i> , 2018, 266, 150-154.	1.4	6
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4248	Comparative study of polytype 2H-MoS <sub>2</sub> and 3R-MoS <sub>2</sub> systems by employing DFT. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2019, 106, 338-345.	1.3	30
4249	$\text{Sr}[\text{B}(\text{OH})_4]_3(\text{IO}_3)_3$ and $\text{Li}_4\text{Sr}_5[\text{B}_{12}\text{O}_{22}(\text{OH})_4]_2(\text{IO}_3)_2$ : two unprecedented metal borate-iodates showing a subtle balance of enlarged band gap and birefringence. <i>Chemical Communications</i> , 2019, 55, 11139-11142.	2.2	29
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4968	First principle calculations of electronic, band structural, and optical properties of Bi <sub>x</sub> Sr <sub>1-x</sub> TiO <sub>3</sub> perovskite. <i>Journal of Physics and Chemistry of Solids</i> , 2019, 127, 107-114.	1.9	27
4969	Structural, spectroscopic, and thermodynamic characterization of ammonium oxalate monohydrate mineral using theoretical solid-state methods. <i>Journal of Physics and Chemistry of Solids</i> , 2019, 125, 31-42.	1.9	14
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4971	Elements (Si, Sn, and Mg) doped $\hat{1}\pm$ -Ga <sub>2</sub> O <sub>3</sub> : First-principles investigations and predictions. <i>Computational Materials Science</i> , 2019, 156, 273-279.	1.4	38
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4988	Antiferromagnetic Slater insulator phase in copper tellurium oxide. <i>Journal of Magnetism and Magnetic Materials</i> , 2020, 495, 165861.	1.0	1
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4990	Structural, optical and electronic properties of CuO and Zn doped CuO: DFT based First-principles calculations. <i>Chemical Physics</i> , 2020, 528, 110536.	0.9	34

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4998	Surface engineering of hollow carbon nitride microspheres for efficient photoredox catalysis. <i>Chemical Engineering Journal</i> , 2020, 381, 122593.	6.6	49
4999	Chalcogenated-Ti <sub>3</sub> C <sub>2</sub> X <sub>2</sub> MXene (X = O, S, Se and Te) as a high-performance anode material for Li-ion batteries. <i>Applied Surface Science</i> , 2020, 501, 144221.	3.1	77
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5020	Density Functional Theory Study of ZnIn <sub>2</sub> S <sub>4</sub> and CdIn <sub>2</sub> S <sub>4</sub> Polymorphs Using Full-Potential Linearized Augmented Plane Wave Method and Modified Becke-Johnson Potential. <i>Physica Status Solidi (B): Basic Research</i> , 2020, 257, 1900485.	0.7	19
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5026	Physico-chemical properties of CrMoN coatings - combined experimental and computational studies. <i>Thin Solid Films</i> , 2020, 693, 137671.	0.8	13

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5034	Rational Localization of Metal Nanoparticles in Yolkâ€­Shell MOFs for Enhancing Catalytic Performance in Selective Hydrogenation of Cinnamaldehyde. <i>ChemSusChem</i> , 2020, 13, 205-211.	3.6	22
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5037	Integrating 2D/2D CdS/Î±-Fe <sub>2</sub> O <sub>3</sub> ultrathin bilayer Z-scheme heterojunction with metallic Î²-NiS nanosheet-based ohmic-junction for efficient photocatalytic H <sub>2</sub> evolution. <i>Applied Catalysis B: Environmental</i> , 2020, 266, 118619.	10.8	199
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5079	Phototherapy ablation of rabbit orthotopic tumors by non-stoichiometric BiPO <sub>4</sub> <sup>x</sup> nanoparticles. <i>Chemical Engineering Journal</i> , 2020, 386, 123961.	6.6	14
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5089	Influence of Au, Cu, Pd added in Ag alloy on stability and electronic structure of Ag/Al interface by first-principles calculations. <i>Materials Today Communications</i> , 2020, 22, 100670.	0.9	6
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5106	NaRb <sub>3</sub> B <sub>6</sub> O <sub>9</sub> (OH) <sub>3</sub> (HCO <sub>3</sub> ): A Borate-Bicarbonate Nonlinear Optical Material. <i>Inorganic Chemistry</i> , 2020, 59, 759-766.	1.9	13
5107	Properties of Si nanostructural modification on Si (111) surface. <i>Chinese Journal of Physics</i> , 2020, 67, 69-78.	2.0	0
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5121	Surface Nonlinear Optics on Centrosymmetric Dirac Nodal-Line Semimetal ZrSiS. <i>Advanced Materials</i> , 2020, 32, e1904498.	11.1	14
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5130	Effect of p-toluenesulfonyl hydrazide on copper corrosion in hydrochloric acid solution. <i>Corrosion Science</i> , 2020, 165, 108363.	3.0	27
5131	Strain-controllable ferromagnetism in Mn-doped AlP semiconductor with constant visible light absorption. <i>Journal of Physics and Chemistry of Solids</i> , 2020, 138, 109274.	1.9	1
5132	Electronic and optical properties of $\text{Tl}_4\text{GeX}_3$ (X = S, Se and Te) compounds for optoelectronics applications: insights from DFT-computations. <i>Journal of Materials Research and Technology</i> , 2020, 9, 413-420.	2.6	6
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5134	$\text{Li}_2\text{CdSiS}_4$ , a promising IR NLO material with a balanced $E_g$ and SHG response originating from the effect of Cd with d10 configuration. <i>Dalton Transactions</i> , 2020, 49, 1975-1980.	1.6	25
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5137	Electrochemical elucidation of $\text{Co}_{0.5}\text{M}_{0.5}\text{V}_2\text{O}_4$ ( $M = \text{Tj, ET, Q, O, O, rg, BT}$ ) <i>Overlock</i> 3349-3360.	3.2	9
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5142	Photocatalytic Application of Two-dimensional Materials-based Heterostructure Based on Molybdenum and Tungsten Disulfides and Gallium Nitride: A Density-Functional Theory Study. <i>Materials Today Communications</i> , 2020, 25, 101646.	0.9	4
5143	Justification of crystal stability and origin of transport properties in ternary half-Heusler ScPtBi. <i>RSC Advances</i> , 2020, 10, 37482-37488.	1.7	10
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5145	The 1H $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"} \rangle \langle \text{mml:mrow} \langle \text{mml:msub} \langle \text{mml:mi} \rangle T \langle \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 1 \langle \text{mml:mn} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \rangle$ dispersion curve of fentanyl citrate to identify NQR parameters. <i>Solid State Nuclear Magnetic Resonance</i> , 2020, 110, 101697.	1.5	2
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5149	$Ba(MoO_{2}F)_{2}(XO_{3})_{2}$ (X = Se and Te): First Cases of Noncentrosymmetric Fluorinated Molybdenum Oxide Selenite/Tellurite Through Unary Substitution for Enlarging Band Gaps and Second Harmonic Generation. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 49812-49821.	4.0	25
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5847	Nonlinear Optical Oxythiophosphate Approaching the Good Balance with Wide Ultraviolet Transparency, Strong Second Harmonic Effect, and Large Birefringence. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 6386-6390.	7.2	49
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6465	2D van der Waals Layered $[\text{C}(\text{NH})_2]_2\text{SO}_3\text{S}$ Exhibits Desirable UV Nonlinear-Optical Trade-Off. <i>Inorganic Chemistry</i> , 2021, 60, 14544-14549.	1.9	18
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7159	Three orders of magnitude two-beam-coupling gain increase from Cu-doped (K <sub>0.5</sub> Na <sub>0.5</sub> ) <sub>0.2</sub> (Sr <sub>0.75</sub> Ba <sub>0.25</sub> ) <sub>0.9</sub> Nb <sub>2</sub> O <sub>6</sub> crystal owing to huge depolarization field-induced surface metallization. European Physical Journal Plus, 2022, 137, 1.	1.2	0
7160	Two novel carbon allotropes with tetragonal symmetry: First-principles calculations. Journal of Solid State Chemistry, 2022, 309, 122971.	1.4	21
7161	Investigating the influence of nano film depositions on the metal surface on the solid-liquid interfacial work function. Surfaces and Interfaces, 2022, 29, 101789.	1.5	1
7162	A study on the electronic properties of A site and B site doped SrTiO <sub>3</sub> for thermoelectric applications using first-principles calculations. Physica Scripta, 2022, 97, 035808.	1.2	1
7163	First-Principles Study on the Half-Metallicity of New MXene Materials Nd <sub>2</sub> NT <sub>2</sub> (T = OH, O, S, F, Cl, and) TJ ETQq1 1 0.784314 pgBT /Overl	1.8	1

#	ARTICLE	IF	CITATIONS
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7165	Understanding the ZIF-L to ZIF-8 transformation from fundamentals to fully costed kilogram-scale production. <i>Communications Chemistry</i> , 2022, 5, .	2.0	45
7166	Abrading bulk metal into single atoms. <i>Nature Nanotechnology</i> , 2022, 17, 403-407.	15.6	102
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7170	Sliding Modulation in Nonlinear Optical Effect in Two-Dimensional van der Waals Cu <sub>2</sub> MoS <sub>4</sub> . <i>ACS Applied Materials &amp; Interfaces</i> , 2022, 14, 9535-9543.	4.0	5
7171	Si-C alloys with direct band gaps for photoelectric application. <i>Vacuum</i> , 2022, 199, 110952.	1.6	16
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7175	NMR Response of the Tetrel Bond Donor. <i>Journal of Physical Chemistry C</i> , 2022, 126, 851-865.	1.5	10
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7177	Few-Layer WS <sub>2</sub> –WSe <sub>2</sub> Lateral Heterostructures: Influence of the Gas Precursor Selenium/Tungsten Ratio on the Number of Layers. <i>ACS Nano</i> , 2022, 16, 1198-1207.	7.3	16
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7180	Ln-Cloridolithates from Ionothermal Synthesis. <i>Inorganic Chemistry</i> , 2021, 60, 19145-19151.	1.9	1
7181	Novel Hydrogen-Bonded Metal-Nucleobase Frameworks for Highly Selective Capture and Separation of Ethane/Propane and Nitrogen from Methane. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0

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7183	Resolving alternative structure determinations of indapamide using <sup>13</sup> C solid-state NMR. Chemical Communications, 2022, 58, 4767-4770.	2.2	2
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7201	Partial reduction of NO to N <sub>2</sub> O on Cu{311}: role of intermediate N <sub>2</sub> O <sub>2</sub> . <i>Catalysis Science and Technology</i> , 2022, 12, 2793-2803.	2.1	2
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7250	Novel Boron Nitride Polymorphs with Graphite-Diamond Hybrid Structure. <i>Chinese Physics Letters</i> , 2022, 39, 036301.	1.3	5
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7817	Characterization of the charge transfer luminescence of the [WO <sub>6</sub> ] <sup>6+</sup> octahedron in Ca <sub>3</sub> WO <sub>6</sub> and the [WO <sub>5</sub> ] <sup>4+</sup> square pyramid in Ca <sub>3</sub> WO <sub>5</sub> Cl <sub>2</sub> . <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 24203-24211.	1.3	2
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8220	$\text{Hf} < \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si98.svg" display="inline" id="d1e2137"> < mml:msub> < mml:mrow /> < mml:mrow> < mml:mn>2</mml:mn> </mml:mrow> </mml:msub> </mml:math> \text{Ge} < \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si99.svg" display="inline"}$		

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8240	Theoretical design of $\text{Mo}_x\text{W}_{1-x}\text{S}_2$ /graphene heterojunction with adjustable band gap: potential candidate materials for next generation of optoelectronic devices. <i>ChemPhysChem</i> , 0, , .	1.0	0
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8242	Solution combustion synthesis of Mg-TiC@NiO nanocomposite and investigation on its metallurgical and biological properties. <i>Journal of Molecular Liquids</i> , 2023, 376, 121487.	2.3	1
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8251	WO <sub>x</sub> nanowire supported ultra-fine Ir-IrO <sub>x</sub> nanocatalyst with compelling OER activity and durability. <i>Chemical Engineering Journal</i> , 2023, 464, 142613.	6.6	9
8252	Raman spectra and vibrational properties of FOX-7 under pressure and temperature: First-principles calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 293, 122489.	2.0	2
8253	Atomic-scale friction of black phosphorus/degraded Cu substrate: A route to robust superlubricity obtained by the critical load. <i>Applied Surface Science</i> , 2023, 619, 156749.	3.1	2
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8256	A comparative study of cubic methylammonium lead iodide (CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> ) perovskite by using density functional theory. <i>Materials Today Communications</i> , 2023, 35, 105814.	0.9	1
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