

# Improved tetrahedron method for Brillouin-zone integr

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Citation Report

#	ARTICLE	IF	CITATIONS
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2	Electronic and Optical Properties of the Group-III Nitrides, their Heterostructures and Alloys. Materials Research Society Symposia Proceedings, 1995, 395, 455.	0.1	20
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1911	Phase stability and thermodynamic modeling of the Re-Ti system supplemented by first-principles calculations. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2012, 38, 71-80.	0.7	11
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1913	Ab initio study of electronic structure and magnetic properties of MFe <sub>3</sub> N (M=Ru and Os). <i>Computational Materials Science</i> , 2012, 65, 6-12.	1.4	8
1914	First principles study of half-metallic ferromagnetism in (N, P, As and Sb) doped alkaline-earth sulfides. <i>Computational Materials Science</i> , 2012, 65, 426-433.	1.4	5
1915	Ab initio study of Ti-C precipitates in hcp titanium: Formation energies, elastic moduli and theoretical diffraction patterns. <i>Computational Materials Science</i> , 2012, 65, 434-441.	1.4	16
1916	Influence of antiphase boundary period parameter $M^2$ on elastic and electronic properties of one dimensional long period structures of Al <sub>3</sub> Ti. <i>Solid State Communications</i> , 2012, 152, 1939-1944.	0.9	7
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1919	First-principles study of electronic, vibrational, elastic, and magnetic properties of FeF <sub>2</sub> as a function of pressure. <i>Physical Review B</i> , 2012, 85,	1.1	50
1920	Chromium Oxide Species Supported on Silica: A Representative Periodic DFT Model. <i>Journal of Physical Chemistry C</i> , 2012, 116, 994-1001.	1.5	55
1921	Linking <sup>31</sup> P Magnetic Shielding Tensors to Crystal Structures: Experimental and Theoretical Studies on Metal(II) Aminotris(methylenephosphonates). <i>Inorganic Chemistry</i> , 2012, 51, 11466-11477.	1.9	19
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1923	A <sub>5</sub> Sn <sub>2</sub> As <sub>6</sub> (A = Sr, Eu). Synthesis, Crystal and Electronic Structure, and Thermoelectric Properties. <i>Inorganic Chemistry</i> , 2012, 51, 5771-5778.	1.9	37

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1925	Exploration of the formation of XLi <sub>3</sub> N <sub>2</sub> compounds (X=Sc-Zn) by means of density functional theory. Physical Review B, 2012, 85, .	1.1	7
1926	Polyolithiated (OLi <sub>2</sub> ) functionalized graphene as a potential hydrogen storage material. Applied Physics Letters, 2012, 101, 243902.	1.5	11
1927	Gaussian charge-transfer charge distributions for non-self-consistent electronic structure calculations. Physical Review B, 2012, 85, .	1.1	3
1928	Lattice dynamics, thermodynamics, and bonding strength of lithium-ion battery materials LiMPO <sub>4</sub> (M = Mn, Fe, Co, and Ni): a comparative first-principles study. Journal of Materials Chemistry, 2012, 22, 1142-1149.	6.7	87
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1931	Magnetic moment of a single vacancy in graphene and semiconducting nanoribbons. Physical Review B, 2012, 86, .	1.1	45
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1934	The mixing of Fe/Co and its effect on the exchange interaction in SmCo <sub>5</sub> /Î±-Fe nanocomposites: A first-principles study. Journal of Applied Physics, 2012, 111, .	1.1	14
1935	First-Principles Calculations on Stabilization of Iron Carbides (Fe <sub>3</sub> C, Fe <sub>5</sub> C <sub>2</sub> , and Î±-Fe <sub>2</sub> C) in Steels by Common Alloying Elements. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2012, 43, 4436-4444.	1.1	52
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1937	Ab initio complex band structure of conjugated polymers: Effects of hybrid density functional theory and calculations of the thermodynamic and kinetic properties of Li <sub>2</sub> GW. Physical Review B, 2012, 85, .	1.1	34
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1939	Suppression of edge magnetism in a titanium-embedded zigzag graphene nanoribbon. Journal of Applied Physics, 2012, 111, 033707.	1.1	11
1940	Adsorption of <sup>l</sup>-DOPA Intercalated in Hydrated Na-Saponite Clay: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry C, 2012, 116, 26414-26421.	1.5	25
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1943	Quantum mechanically guided design of $\text{Co}_{43}\text{Fe}_{20}\text{Ta}_{5.5}\text{X}_{31.5}$ ( $\text{X}=\text{B}, \text{Si}, \text{P}, \text{S}$ ) metallic glasses. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 175402.	0.7	5
1944	Elastic and electronic properties of $\text{Mg}_{12}\text{RE}$ ( $\text{RE} = \text{Ce}, \text{Pr}$ and $\text{Nd}$ ) phases. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2012, 20, 035018.	0.8	50
1945	Diverse Closed Cavities in Condensed Rare Earth Metal-Chalcogenide Matrixes: $\text{Cs}[\text{Lu}_7\text{Q}_{11}]$ and $(\text{ClCs}_6)[\text{RE}_{21}\text{Q}_{34}]$ ( $\text{RE} = \text{Tm}, \text{Yb}$ )	1.0	7
1946	Structures and properties of the ternary thallium chalcogenides $\text{Tl}_2\text{MQ}_3$ ( $\text{M} = \text{Zr}, \text{Hf}$ ; $\text{Q} = \text{S}, \text{Se}$ ). <i>Dalton Transactions</i> , 2012, 41, 9646.	1.6	8
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1953	Polymorphism of $\text{Li}_2\text{Zn}_3$ . <i>Acta Crystallographica Section B: Structural Science</i> , 2012, 68, 34-39.	1.8	11
1954	Elastic moduli of advanced orthorhombic binary and ternary metal ( $\text{V}, \text{Ta}, \text{Nb}$ ) nitrides with the $\text{U}_2\text{S}_3$ structure. <i>Physica Status Solidi (B): Basic Research</i> , 2012, 249, 1020-1026.	0.7	7
1955	Barium Peroxide: a Simple Test Case for First-Principles Investigations on the Temperature Dependence of Solid-State Vibrational Frequencies. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2012, 638, 1403-1406.	0.6	8
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1957	Migration of nitrogen in hexagonal $\text{Ge}_2\text{Sb}_2\text{Te}_5$ : An <i>ab initio</i> study. <i>Physica Status Solidi - Rapid Research Letters</i> , 2012, 6, 108-110.	1.2	2
1958	<i>Ab initio</i> electron energy-loss spectra and depolarization effects: Application to carbon nanotubes. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 2171-2184.	1.0	1
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1962	<i>Ab initio</i> modeling of the structural, electronic, and optical properties of $A_{x-1}B_2$ and $A_{x-1}B_3$ compounds. Physical Review B, 2012, 85, 045111.	1.1	121
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1965	Electronic structure and thermodynamics of V <sub>2</sub> O <sub>3</sub> polymorphs. Journal of Computational Chemistry, 2012, 33, 2102-2107.	1.5	18
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1967	A First-Principles Investigation of the Compositional Dependent Properties of Magnetic Shape Memory Heusler Alloys. Advanced Engineering Materials, 2012, 14, 530-546.	1.6	54
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1970	The Role of Effective Mass of Carrier in the Photocatalytic Behavior of Silver Halide-Based Ag@AgX (X=Cl, Br, I): A Theoretical Study. ChemPhysChem, 2012, 13, 2304-2309.	1.0	99
1971	Mineral-organic interfacial processes: potential roles in the origins of life. Chemical Society Reviews, 2012, 41, 5502.	18.7	205
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1973	Electronic structure and magnetic properties of Sr <sub>1-x</sub> MnO <sub>3</sub> and MnO <sub>x</sub> . Physical Review B, 2012, 85, 115111.	1.1	31
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1979	The structural, electronic, elastic and optical properties of AlCu(Se <sup>1+</sup> Te <sup>-2</sup> ) <sub>2</sub> compounds from first-principle calculations. <i>Current Applied Physics</i> , 2012, 12, 373-379.	1.1	9
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1981	Structural stability, mechanical property and elastic anisotropy of TiAl-H system. <i>International Journal of Hydrogen Energy</i> , 2012, 37, 2676-2684.	3.8	27
1982	Stability of erbium hydrides studied by DFT calculations. <i>International Journal of Hydrogen Energy</i> , 2012, 37, 4246-4253.	3.8	12
1983	Atomistic study of LaNbO <sub>4</sub> ; surface properties and hydrogen adsorption. <i>International Journal of Hydrogen Energy</i> , 2012, 37, 6674-6685.	3.8	13
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1993	Theoretical investigations of NiTiSn and CoVSn compounds. <i>Journal of Physics and Chemistry of Solids</i> , 2012, 73, 975-981.	1.9	44
1994	Electronic states of metal (Cu, Ag, Au) atom on CeO <sub>2</sub> (111) surface: The role of local structural distortion. <i>Journal of Power Sources</i> , 2012, 197, 28-37.	4.0	46
1995	Structural, energetic and thermodynamic analyses of Ca(BH <sub>4</sub> ) <sub>2</sub> ·2NH <sub>3</sub> from first principles calculations. <i>Journal of Solid State Chemistry</i> , 2012, 185, 206-212.	1.4	10

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1997	Synthesis and structural characterization of the ternary Zintl phases AE <sub>3</sub> Al <sub>2</sub> Pn <sub>4</sub> and AE <sub>3</sub> Ga <sub>2</sub> Pn <sub>4</sub> (AE=Ca, Sr, Ba, Eu; Pn=P, As). Journal of Solid State Chemistry, 2012, 188, 59-65.	1.4	40
1998	Ideal strength and deformation-induced phase transformation of hcp metals Re, Ru, and Os: A first-principles study. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2012, 534, 353-364.	2.6	12
1999	Mechanical properties and work function of L21 structure AlCu <sub>2</sub> X (X=Ti, Mn, Zr, or Hf) intermetallics. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2012, 545, 13-19.	2.6	11
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2010	Electronic structure and properties of BaAlGe and SrAlGe. Physica C: Superconductivity and Its Applications, 2012, 476, 54-58.	0.6	6
2011	Formation energies and swelling of uranium dioxide by point defects. Physics Letters, Section A: General, Atomic and Solid State Physics, 2012, 376, 1499-1505.	0.9	8
2012	Phase stability, mechanical property, and electronic structure of an Mg-Ca system. Journal of the Mechanical Behavior of Biomedical Materials, 2012, 8, 154-164.	1.5	42
2013	Interlayer exchange coupling in multilayered Co/Os. Journal of Magnetism and Magnetic Materials, 2012, 324, 146-153.	1.0	0



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2015	Effect of Au proximity on the LSMO surface: An ab initio study. Journal of Magnetism and Magnetic Materials, 2012, 324, 2659-2663.	0.2	9
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2024	A first-principles study on magnetocrystalline anisotropy at interfaces of Fe with non-magnetic metals. Journal of Applied Physics, 2013, 113, 233908.	1.1	32
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2029	Correlations between Chemical Bonding and Magnetic Exchange Interactions: Synthesis, Crystal Structures, and Magnetic Properties of the New Family $\text{RE}_2\text{AlGe}_2$ ( $\text{RE} = \text{Tb, Tm, Lu}$ ). Inorganic Chemistry, 2013, 52, 5307-5315.	1.4	24
2030	First-principles calculations of finite-temperature elastic properties of $\text{Ti}_2\text{AlX}$ ( $X = \text{C or N}$ ). Computational Materials Science, 2013, 79, 296-302.	1.9	50
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2033	The migration and formation energies of N-interstitials near [001] Fe surfaces: an ab initio study. <i>Journal of Materials Science</i> , 2013, 48, 6542-6548.	1.7	2
2034	Hydrogen trapping in $\delta$ -Pu: insights from electronic structure calculations. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 265001.	0.7	12
2035	Crystallinity-dependent substitutional nitrogen doping in ZnO and its improved visible light photocatalytic activity. <i>Journal of Colloid and Interface Science</i> , 2013, 400, 18-23.	5.0	61
2036	A Molecular Picture of the Adsorption of Glycine in Mesoporous Silica through NMR Experiments Combined with DFT-D Calculations. <i>Journal of Physical Chemistry C</i> , 2013, 117, 4104-4114.	1.5	60
2037	Theoretical investigation of the Al-Cr-B orthorhombic ternary compounds. <i>Computational and Theoretical Chemistry</i> , 2013, 1020, 51-56.	1.1	18
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2041	Theoretical assessment of graphene-metal contacts. <i>Journal of Chemical Physics</i> , 2013, 138, 244701.	1.2	58
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2993	Sulfur to oxygen substitution in $\text{BiOCuSe}$ and its effect on the thermoelectric properties. <i>Journal of Materials Chemistry A</i> , 2016, 4, 13859-13865.	5.2	14
2994	Carbon-rich icosahedral boron carbides beyond $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi mathvariant="normal"} \rangle \text{B} \langle / \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 4 \langle / \text{mml:mn} \rangle \langle / \text{mml:msub} \rangle \langle \text{mml:mi mathvariant="normal"} \rangle \text{C} \langle / \text{mml:mi} \rangle \langle / \text{mml:mrow} \rangle \langle / \text{mml:math} \rangle$ and their thermodynamic stabilities at high temperature and pressure from first principles. <i>Physical Review B</i> , 2016, 94, .	1.1	21
2995	A Density Functional Theory Study of the Ionic and Electronic Transport Mechanisms in $\text{LiFeBO}_3$ Battery Electrodes. <i>Journal of Physical Chemistry C</i> , 2016, 120, 18355-18364.	1.5	24
2996	First-principles investigation of phase stability, elastic and thermodynamic properties in $\text{L12 Co}_3(\text{Al,Mo,Nb})$ phase. <i>Intermetallics</i> , 2016, 78, 1-7.	1.8	22
2997	Group Additivity for Thermochemical Property Estimation of Lignin Monomers on $\text{Pt}(111)$ . <i>Journal of Physical Chemistry C</i> , 2016, 120, 19234-19241.	1.5	18
2998	Metal Nitrides Grown from $\text{Ca/Li}$ Flux: $\text{Ca}_6\text{Te}_3\text{N}_2$ and New Nitridoferrate(I) $\text{Ca}_6(\text{Li}_x\text{Fe}_{1-x})\text{Te}_2\text{N}_3$ . <i>Journal of the American Chemical Society</i> , 2016, 138, 10636-10644.	6.6	10
2999	Localization of the interband transitions in the bulk of the Brillouin zone of $\text{III-V}$ compound crystals. <i>Semiconductors</i> , 2016, 50, 572-578.	0.2	2
3000	$\langle i \rangle \text{Ab initio} \langle /i \rangle$ electron mobility and polar phonon scattering in $\text{GaAs}$ . <i>Physical Review B</i> , 2016, 94, .	1.1	142
3001	Hydration in silica based mesoporous materials: a DFT model. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 32962-32972.	1.3	44
3002	Impact of lattice dynamics on the phase stability of metamagnetic $\text{FeRh}$ : Bulk and thin films. <i>Physical Review B</i> , 2016, 94, .	1.1	44
3003	Electron-Hybridization-Induced Enhancement of Photoactivity in Indium-Doped $\text{Co}_3\text{O}_4$ . <i>Journal of Physical Chemistry C</i> , 2016, 120, 28983-28991.	1.5	4
3004	High-throughput combinatorial study of the effect of $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mi} \rangle \text{M} \langle / \text{mml:mi} \rangle \langle / \text{mml:math} \rangle$ site alloying on the solid solution behavior of $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{M} \langle / \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 2 \langle / \text{mml:mn} \rangle \langle / \text{mml:mrow} \rangle \langle / \text{mml:math} \rangle$ phases. <i>Physical Review B</i> , 2016, 94, .	1.1	38
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3006	Conflict between the Electronic Factors and Structure-Directing Rules in the Intergrowth Structure of $\text{Ca}_4\text{Ag}_2\langle i \rangle \text{x} \langle /i \rangle \text{Ge}_4\langle i \rangle \text{x} \langle /i \rangle$ with $\langle i \rangle \text{x} \langle /i \rangle = 1/2$ . <i>Crystal Growth and Design</i> , 2016, 16, 5946-5953.	1.4	3
3007	Block antiferromagnetism and possible ferroelectricity in $\text{KFe}_2\text{Se}_2$ . <i>Physica Status Solidi - Rapid Research Letters</i> , 2016, 10, 757-761.	1.2	6
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3009	Yttrium-Doped $\text{Sb}_2\text{Te}_3$ : A Promising Material for Phase-Change Memory. <i>ACS Applied Materials &amp; Interfaces</i> , 2016, 8, 26126-26134.	4.0	99

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3011	Characterization of high-performance organic dyes for dye-sensitized solar cell: a DFT/TDDFT study. Canadian Journal of Chemistry, 2016, 94, 1109-1118.	0.6	7
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3044	Archimedean (4,8)-tessellation of haeckelite ultrathin nanosheets composed of boron and aluminum-group V binary materials. Nanoscale, 2016, 8, 19287-19301.	2.8	12

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3263	RhCd <sub>9</sub> Ir (a <sup>~</sup> 1.18% <sup>~</sup> a <sup>~</sup> 0.29) a $\bar{1}$ -brass related cubic giant cell structure. Zeitschrift Fur Kristallographie - Crystalline Materials, 2017, 232, 611-617.	0.4	3
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3276	Effects of hole doping and strain on magnetism in buckled phosphorene and arsenene. 2D Materials, 2017, 4, 025107.	2.0	40
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3315	Low temperature synthesis of ternary metal phosphides using plasma for asymmetric supercapacitors. <i>Nano Energy</i> , 2017, 35, 331-340.	8.2	324



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3355	Atomic oxygen adsorption on Pb(1 0 0). <i>European Physical Journal B</i> , 2017, 90, 1.	0.6	0
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4000	The effect of grain boundary on the visible light absorption of BaTi <sub>1-x</sub> [Ni <sub>1/2</sub> Nb <sub>1/2</sub> ] <sub>x</sub> O <sub>3</sub> ferroelectric ceramics. Journal of the American Ceramic Society, 2019, 102, 7405-7413.	1.9	16
4001	Structural, Electronic, and Magnetic Properties of Hard Magnetic SmNi <sub>2</sub> Fe Compound: a DFT Study. Journal of Superconductivity and Novel Magnetism, 2019, 32, 3901-3905.	0.8	3
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4004	Evidence for Fe-Si-O liquid immiscibility at deep Earth pressures. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 10238-10243.	3.3	24
4005	S <sup>d</sup> -Doped Graphene <sup>e</sup> -Regional Nucleation Mechanism for Dendrite <sup>e</sup> -Free Lithium Metal Anodes. <i>Advanced Energy Materials</i> , 2019, 9, 1804000.	10.2	74
4006	Structural and magnetic properties of YCo <sub>4</sub> B compound at high pressures. <i>Intermetallics</i> , 2019, 110, 106489.	1.8	2
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4009	Distinction between Intrinsic and X-ray-Induced Oxidized Oxygen States in Li-Rich 3d Layered Oxides and LiAlO <sub>2</sub> . <i>Journal of Physical Chemistry C</i> , 2019, 123, 13201-13207.	1.5	33
4010	Nonlinear elasticity of $\epsilon$ -Fe: The pressure effect. <i>Physical Review B</i> , 2019, 99, .	1.1	2
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4012	Electronic Metal <sup>e</sup> -Support Interaction To Modulate MoS <sub>2</sub> -Supported Pd Nanoparticles for the Degradation of Organic Dyes. <i>ACS Applied Nano Materials</i> , 2019, 2, 3385-3393.	2.4	43
4013	A practical ansatz for evaluating the electronic friction tensor accurately, efficiently, and in a nearly black-box format. <i>Journal of Chemical Physics</i> , 2019, 150, 164105.	1.2	9
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4015	Thermodynamic Stability, Thermoelectric, Elastic and Electronic Structure Properties of ScMN <sub>2</sub> -Type (M = V, Nb, Ta) Phases Studied by <i>ab initio</i> Calculations. <i>Condensed Matter</i> , 2019, 4, 36.	0.8	2
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4017	First-principles study of structural stability, electronic properties and lattice thermal conductivity of KAgX (X = S, Se, Te). <i>European Physical Journal B</i> , 2019, 92, 1.	0.6	8
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4019	<i>Ab initio</i> study on structural and electronic properties of ReOFeAs (Re: La, Sm, Nd, Ce, Gd) under hydrostatic pressure. <i>Journal of Physics Communications</i> , 2019, 3, 015013.	0.5	1
4020	<i>Resolving the FCC/FCC interface of the</i> $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \text{altimg="si1.svg"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle^3 \langle \text{mml:mi} \rangle \langle \text{mml:mo} \rangle ' \langle \text{mml:mo} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle$ Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 3-8 Td (altimg="si2.svg") precipitate phase in aluminium. <i>Acta Materialia</i> , 2019, 174, 116-130.	3.8	20

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4034	Effects of high pressure on $\text{ScMN}_2$ -type (M = V, Nb, Ta) phases studied by density functional theory. <i>Results in Physics</i> , 2019, 13, 102293.	2.0	1
4035	Coinage Metal-Sulfur Complexes: Stability on Metal(111) Surfaces and in the Gas Phase. <i>Journal of Physical Chemistry C</i> , 2019, 123, 12954-12965.	1.5	5
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4040	Design and synthesis of Ga-doped ZSM-22 zeolites as highly selective and stable catalysts for <i>n</i> -dodecane isomerization. <i>Catalysis Science and Technology</i> , 2019, 9, 2812-2827.	2.1	22
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4043	Intermetallic Differences at CdSâ€“Metal (Ni, Pd, Pt, and Au) Interfaces: From Single-Atom to Subnanometer Metal Clusters. <i>Journal of Physical Chemistry C</i> , 2019, 123, 9298-9310.	1.5	7
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4048	Advances in Sustainable Catalysis: A Computational Perspective. <i>Frontiers in Chemistry</i> , 2019, 7, 182.	1.8	36
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4051	An insight into optical properties of Pb:CdS system (a theoretical study). <i>Materials Research Express</i> , 2019, 6, 065904.	0.8	8
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4053	Tuning the Magnetic Anisotropy of NiPtMnGa by Substitution and Epitaxial Strain. <i>IEEE Transactions on Magnetics</i> , 2019, 55, 1-4.	1.2	2
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4055	Strain-induced indirect-to-direct bandgap transition in an np-type LaAlO <sub>3</sub> /SrTiO <sub>3</sub> (110) superlattice. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7075-7082.	1.3	2
4056	Magnetic and electronic properties of Cr <sub>2</sub> Ge <sub>2</sub> Te <sub>6</sub> monolayer by strain and electric-field engineering. <i>Applied Physics Letters</i> , 2019, 114, .	1.5	69

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4070	First-Principle Studies of Ferrimagnetic Double Perovskite Ca <sub>2</sub> FeMoO <sub>6</sub> Compound. Journal of Superconductivity and Novel Magnetism, 2019, 32, 2913-2922.	0.8	2
4071	Phase Segregation, Transition, or New Phase Formation of Plutonium Dioxide: The Roles of Transition Metals. Inorganic Chemistry, 2019, 58, 4350-4364.	1.9	21
4072	Strain Modulated Optoelectronic Properties of CdO Monolayer. Journal of Electronic Materials, 2019, 48, 3963-3969.	1.0	15
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4077	Li <sub>20</sub> Mg <sub>6</sub> Cu <sub>13</sub> Al <sub>42</sub> : a new ordered quaternary superstructure to the icosahedral $T\bar{1}$ -Mg <sub>32</sub> (Zn,Al) <sub>49</sub> phase with fullerene-like Al <sub>60</sub> cluster. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2019, 75, 168-174.	0.5	4
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4085	Study of elastic, structural, electronic, magnetic, and topological properties of $\hat{1}$ -Fe <sub>2</sub> C carbide under pressure. <i>Journal of Physics and Chemistry of Solids</i> , 2019, 131, 196-212.	1.9	6
4086	Equation of state of boron nitride combining computation, modeling, and experiment. <i>Physical Review B</i> , 2019, 99, .	1.1	28
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4090	Intrinsic magnetic properties of SmFe <sub>12</sub> V alloys with reduced V-concentration. <i>Journal of Alloys and Compounds</i> , 2019, 786, 969-974.	2.8	45
4091	Boosting photochemical activity by Ni doping of mesoporous CoO nanoparticle assemblies. <i>Inorganic Chemistry Frontiers</i> , 2019, 6, 765-774.	3.0	10
4092	High Thermoelectric Power Factor in IntermetallicCoSiArising from Energy Filtering of Electrons by Phonon Scattering. <i>Physical Review Applied</i> , 2019, 11, .	1.5	31

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4116	Mechanisms of alumina growth <i>via</i> atomic layer deposition on nickel oxide and metallic nickel surfaces. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 24543-24553.	1.3	5
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4119	Two-dimensional ZrB <sub>2</sub> C <sub>2</sub> with multiple tunable Dirac states. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 24212-24217.	1.3	10
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4133	Thermotropic liquid crystal (5CB) on two-dimensional materials. <i>Physical Review E</i> , 2019, 100, 062701.	0.8	7
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4145	First-principles study of thermophysical properties of interaction layer products in U-Mo/Al dispersion fuel. <i>Journal of Nuclear Materials</i> , 2019, 513, 94-101.	1.3	1
4146	Predicting partial atomic charges in siliceous zeolites. <i>Microporous and Mesoporous Materials</i> , 2019, 277, 184-196.	2.2	8

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4161	Enhancement of monolayer SnSe light absorption by strain engineering: A DFT calculation. <i>Chemical Physics</i> , 2019, 521, 5-13.	0.9	54
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4167	Impurity induced cross luminescence in KMgCl <sub>3</sub> : an <i>ab initio</i> study. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 115501.	0.7	5
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4196	Thermodynamic and kinetic roles of H <sub>2</sub> in structure evolution of urchin-like Co: A density functional theory study. <i>Particuology</i> , 2020, 48, 2-12.	2.0	2
4197	Reshaping of Rh nanoparticles in operando conditions. <i>Catalysis Today</i> , 2020, 350, 184-191.	2.2	3
4198	An ab initio study of filled skutterudites EuOs <sub>4</sub> Sb <sub>12</sub> . <i>Indian Journal of Physics</i> , 2020, 94, 341-351.	0.9	2
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4200	Cobalt-nickel bimetallic Fischer-Tropsch catalysts: A combined theoretical and experimental approach. <i>Catalysis Today</i> , 2020, 342, 88-98.	2.2	27

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4238	Structural and mechanical properties of ternary MgCaSi phase: A study by density functional theory. Journal of Chemical Research, 2020, 44, 50-59.	0.6	2
4239	First-principles calculations to investigate structural and thermodynamic properties of Ni <sub>2</sub> LaZ (Z = As, Sb, Bi) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	0.9	121
4240	Li <sub>2</sub> CdSi <sub>4</sub> S <sub>4</sub> , a promising IR NLO material with a balanced E <sub>g</sub> and SHG response originating from the effect of Cd with d <sub>10</sub> configuration. Dalton Transactions, 2020, 49, 1975-1980.	1.6	25
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4242	First-principles study of FeNi <sub>1-x</sub> Cr <sub>x</sub> (0 ≤ x ≤ 1) disordered alloys from special quasirandom structures. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2020, 71, 102007.	0.7	7
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4251	Pressure-Induced Metallization of Diamond at Room Temperature. Journal of Superhard Materials, 2020, 42, 177-189.	0.5	1
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4253	Phonon-limited electron mobility in Si, GaAs, and GaP with exact treatment of dynamical quadrupoles. Physical Review B, 2020, 102, .	1.1	47
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