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## Universal elastic anisotropy index

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1010	Structural stability and mechanical properties of $\text{Co}_3(\text{Al}, \text{M})$ ( $\text{M} = \text{Ti}, \text{V}, \text{Cr}, \text{Zr}, \text{Nb}, \text{Mo}, \text{Hf}, \text{Ta}, \text{W}$ ) compounds. <b>2018</b> , 148, 27-37	17
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1007	Elastic anisotropies and thermal conductivities of $\text{WB}_2$ diborides in different crystal structures: A first-principles calculation. <b>2018</b> , 747, 905-915	37
1006	Theoretical investigations of $\text{Ge}_{1-x}\text{Sn}_x$ alloys ( $x = 0, 0.333, 0.667, 1$ ) in $\text{P4}_2/\text{ncm}$ phase. <b>2018</b> , 53, 9611-9626	23
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1003	First-principles predictions on structural, elastic and half-metallic properties of $\text{Fe}_2\text{LiAs}$ Heusler compound. <b>2018</b> , 458, 235-240	5
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976	Elastic anisotropy and thermal properties of extended linear chain compounds MV <sub>2</sub> Ga <sub>4</sub> (M = Sc, Zr, Hf) from ab-initio calculations. <b>2018</b> , 4, 529-539	6
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966	Mechanical and Dynamic Stability of Complete and Nonstoichiometric 3C-SixCy from Ab Initio Calculations. <b>2018</b> , 60, 2012-2018	
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961	Elasticity, lattice dynamics and ideal strengths of $\text{USi}_3$ and $\text{U}_3\text{Si}$ via first principles calculations. <b>2018</b> , 512, 407-416	3
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928	Machine Learning Enabled Computational Screening of Inorganic Solid Electrolytes for Suppression of Dendrite Formation in Lithium Metal Anodes. <b>2018</b> , 4, 996-1006	92

927	Prediction of structural properties of protactinium pentoxide $\text{Pa}_2\text{O}_5$ by first-principles calculations. <b>2018</b> , 5, 105903	1
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925	Anisotropy of mechanical and thermal properties of perovskite $\text{LaYbO}_3$ : first-principles calculations. <b>2018</b> , 98, 2917-2929	3
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910	First-principle investigation of hydrogen solubility and diffusivity in transition metal-doped vanadium membranes and their mechanical properties. <b>2019</b> , 805, 747-756	17

909	Elastic anisotropies and thermal properties of cubic TMIr (TM=Sc, Y, Lu, Ti, Zr and Hf): A DFT calculation. <b>2019</b> , 6, 086574	18
908	Electronic structure, elastic and thermal transport properties of thorium monocarbide based on first-principles study. <b>2019</b> , 524, 141-148	4
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902	First-principles study on the mechanical properties of interstitial solid solution Aluminum-Boron alloy. <b>2019</b> , 170, 109159	2
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866	Mechanical and thermodynamic properties of two-dimensional monoclinic Ga <sub>2</sub> O <sub>3</sub> . <b>2019</b> , 184, 108197	17
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862	Determination of representative volume elements for small cracks in heterogeneous, linear-elastic domains. <b>2019</b> , 220, 106643	2
861	First Brillouin zone-centre phonon frequencies and elastic stiffness of the Ln <sub>2</sub> Hf <sub>2</sub> O <sub>7</sub> (Ln = La, Nd, Sm and Eu) pyrochlore. <b>2019</b> , 21, e00428	0
860	Characterization of the orthotropic viscoelastic tensor of composites using the Ultrasonic Polar Scan. <b>2019</b> , 230, 111499	8
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858	Theoretical prediction of new structure, mechanical properties, anisotropy in elasticity and thermodynamic properties of Mo <sub>3</sub> Ge material. <b>2019</b> , 170, 108978	20
857	First-principles study of structural, electronic, elastic, thermodynamic and optical properties of LuPdBi half-Heusler compound. <b>2019</b> , 33, 1950378	13
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684	First principles investigations of structural, elastic, mechanical, electronic and optical properties of triple perovskite Ba <sub>2</sub> K <sub>2</sub> Te <sub>2</sub> O <sub>9</sub> . <b>2020</b> , 596, 412404	8
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677	Physical and optoelectronic features of lead-free A <sub>2</sub> AgRhBr <sub>6</sub> (A = Cs, Rb, K, Na, Li) with halide double perovskite composition. <b>2020</b> , 8, 12968-12983	9
676	Insight of structural stability, elastic anisotropies and thermal conductivities of Y, Sc doped Mg <sub>2</sub> Pb from first-principles calculations. <b>2020</b> , 756, 137833	6

675	Extensive investigation of structural, electronic, optical, and thermoelectric properties of hybrid perovskite (CH <sub>3</sub> NH <sub>3</sub> PbBr <sub>3</sub> ) with mechanical stability constants. <b>2020</b> , 44, 11614-11628	11
674	Elastic properties and anisotropic behavior of structure-H (sH) gas hydrate from first principles. <b>2020</b> , 227, 115948	12
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660	Chemically stable new MAX phase VSnC: a damage and radiation tolerant TBC material.. <b>2020</b> , 10, 43783-43798 <sub>1,2</sub>	
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650	Study of structural, elastic, electronic, and vibrational properties of MRhO (M = Cd and Zn) spinels: DFT-based calculations. <b>2020</b> , 26, 140	1
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648	A comparative study of integration algorithms for finite single crystal (visco-)plasticity. <b>2020</b> , 180, 105740	4
647	Phonon thermodynamics and elastic behavior of GaAs at high temperatures and pressures. <b>2020</b> , 101,	1
646	Reactive elements dependence of elastic properties and stacking fault energies of $\epsilon$ -Ni, $\delta$ -Ni <sub>3</sub> Al and $\epsilon$ -NiAl. <b>2020</b> , 843, 155799	7
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643	First-principles prediction of structural, mechanical and thermal properties of perovskite BaZrS <sub>3</sub> . <b>2020</b> , 93, 1	2
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639	Investigation on the stability, electronic, optical, and mechanical properties of novel calcium carbonate hydrates via first-principles calculations. <b>2020</b> , 120, e26219	3
638	Effective Anisotropic Elastic and Plastic Yield Properties of Periodic Foams Derived from Triply Periodic Schoenfl-WP Minimal Surface. <b>2020</b> , 146, 04020030	11
637	Defective structures in FeCrAl alloys from first principles calculations. <b>2020</b> , 59, 046003	5
636	A comparative theoretical investigation of optoelectronic and mechanical properties of KYS2 and KLaS2. <b>2020</b> , 113, 105048	5
635	The magnesium uranyl tricarbonat octadecahydrate mineral, bayleyite: Periodic DFT study of its crystal structure, hydrogen bonding, mechanical properties and infrared spectrum. <b>2020</b> , 234, 118216	5
634	Research on Simulation, Experiment and Evaluation Method of Different Ratio Gd Doped AgSnO <sub>3</sub> Contact Material. <b>2020</b> , 8, 55471-55482	1
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631	Pressure effect on structural stability and optical absorption of triclinic NbS <sub>3</sub> from DFT and many-body perturbation calculations. <b>2020</b> , 93, 1	2
630	Evaluation of stabilities and thermophysical properties of Si-Sr intermetallics based on first-principles analysis. <b>2020</b> , 18, 103207	1
629	First-principles calculations of mechanical, electronic and optical properties of a new imidooxonitridophosphate. <b>2020</b> , 538, 110917	1
628	First-principles calculations on two superhard BCN allotropes: P3 <sub>1</sub> m1-BCN and I41md-BCN. <b>2020</b> , 184, 109869	1
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623	Insight into structural, electronic, elastic and thermal properties of A15-type Nb <sub>3</sub> X (X = Si, Ge, Sn and Pb) compounds. <b>2020</b> , 25, 101410	9
622	First principles calculations of structural, electronic and optical properties MoX <sub>2</sub> (X = S, Se) metal dichalcogenides and their nano-layers. <b>2020</b> , 503, 166572	5

621	On Prediction of a Novel Chiral Material YHO(OH): A Hydroxyhydride Holding Hydridic and Protonic Hydrogens. <b>2020</b> , 13,	0
620	First-principles study of phase transition, elastic and thermodynamic properties of ZnSe at high pressure. <b>2020</b> , 10, 3265	1
619	Effect of Zr concentration on the mechanical and thermodynamic properties of NbIr <sub>3</sub> intermetallic compounds from theoretical estimations. <b>2020</b> , 100, 1550-1568	
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617	Uranosphaerite: Crystal structure, hydrogen bonding, mechanics, infrared and Raman spectroscopy and thermodynamics. <b>2020</b> , 141, 109400	6
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615	Structural, elastic, electronic, bonding, and optical properties of topological CaSn <sub>3</sub> semimetal. <b>2020</b> , 829, 154509	36
614	First-principles study of mechanical and thermodynamic properties of intermetallic Pt <sub>3</sub> M (M = Al, Hf, Zr, Co, Y, Sc). <b>2020</b> , 23, e00462	6
613	First-principles study of phase stability and temperature-dependent mechanical properties of (Cr, M) <sub>23</sub> C <sub>6</sub> (M = Fe, Mo) phases. <b>2020</b> , 824, 153948	11
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607	Seismic Wave Speeds Derived from Nuclear Resonant Inelastic X-ray Scattering for Comparison with Seismological Observations. <b>2020</b> , 10, 331	1
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604	Research on Mechanical Properties of High-Pressure Anhydrite Based on First Principles. <b>2020</b> , 10, 240	2

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595	Pressure-induced structure, electronic, thermodynamic and mechanical properties of Ti <sub>2</sub> AlNb orthorhombic phase by first-principles calculations. <b>2021</b> , 40, 1-11	6
594	Bayesian estimation of single ply anisotropic elastic constants from spherical indentations on multi-laminate polymer-matrix fiber-reinforced composite samples. <b>2021</b> , 56, 1575-1586	6
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592	The vibrational, thermodynamic and mechanical properties of four types HMX based on the first-principles study. <b>2021</b> , 39, 125-169	8
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590	High-pressure structural, lattice dynamics, and electronic properties of beryllium aluminate studied from first-principles theory. <b>2021</b> , 26, 101801	4
589	Electronic, optical and elastic properties of cubic zirconia (c-ZrO <sub>2</sub> ) under pressure: A DFT study. <b>2021</b> , 604, 412462	4
588	Strain Engineering of Metal Halide Perovskites on Coupling Anisotropic Behaviors. <b>2021</b> , 31, 2006243	31
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582	Quantum electronic pressure and crystal compressibility for magnesium diboride under simulated compression. <b>2021</b> , 26, 101952	2
581	The structural, mechanical and electronic properties of NbXSi (X=Fe, Co, Ni, Ru, Rh, Pd, Os, Ir and Pt) compounds from first-principles calculations. <b>2021</b> , 259, 124029	4
580	Finite element modeling of fretting wear in anisotropic composite coatings: Application to HVOF Cr <sub>3</sub> C <sub>2</sub> NiCr coating. <b>2021</b> , 155, 106765	8
579	Newly Synthesized Ta-Based MAX Phase (Ta <sub>1-x</sub> Hfx) <sub>4</sub> AlC <sub>3</sub> and (Ta <sub>1-x</sub> Hfx) <sub>4</sub> Al <sub>0.5</sub> Sn <sub>0.5</sub> C <sub>3</sub> (0 ≤ x ≤ 0.25) Solid Solutions: Unravelling the Mechanical, Electronic, and Thermodynamic Properties. <b>2021</b> , 258, 2000307	6
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577	First-Principles study of structural, elastic and electronic properties for the KT-GaBP2 semiconductor under pressure. <b>2021</b> , 123, 105585	
576	Development and characterization of Al <sub>3</sub> Al <sub>3</sub> Ni <sub>3</sub> Bn metal matrix composite. <b>2021</b> , 259, 124027	5
575	The mechanical and thermal properties of (Th,U)Si compounds: A systematic density functional theory research. <b>2021</b> , 188, 110148	4
574	Theoretic quantum analysis of mechanical and electronic properties of TiAl-M (M = Mo, W, Cu and Zn). <b>2021</b> , 121, e26590	1
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572	Stability, mechanical, anisotropic and electronic properties of oP8 carbon: A superhard carbon allotrope in orthorhombic phase. <b>2021</b> , 294, 121894	24
571	Microscale bonding mechanism of Mg alloy and steel welded joint with nanoscale Al-based intermetallic compound interface layers. <b>2021</b> , 26, 101924	0
570	First principles prediction of exceptional mechanical and electronic behaviour of Titanite (CaTiSiO <sub>5</sub> ). <b>2021</b> , 15, 100964	2
569	A multiscale modeling of damage accumulation and permeability variation in shale rocks under mechanical loading. <b>2021</b> , 198, 108123	3
568	A predicted non-layered phase of In <sub>2</sub> Se <sub>3</sub> by first principles. <b>2021</b> , 325, 114159	1

567	First-principles investigations on the ground-state bulk properties and lattice constant dependent half-metallic ferrimagnetism of Mn <sub>2</sub> NbSi full-Heusler compound. <b>2021</b> , 121, e26566	0
566	Elastic anisotropies and thermodynamic properties of metal dodecaborides under high pressure. <b>2021</b> , 154, 106346	3
565	Effects of Pressure on the Structural, Mechanical, and Electronic Properties and Debye Temperature of Pd-Based Alloy: First-Principles Calculation. <b>2021</b> , 258, 2000490	
564	Phase-change regulation criterion based on size-dependent lattice distortion rate and born theory for VO <sub>2</sub> nanomaterials. <b>2021</b> , 47, 3232-3237	2
563	Elastic, Electronic, Optical, Thermodynamic, and Superconducting Properties of CaMSi <sub>3</sub> (M = Ir, Pt) and LaMSi <sub>3</sub> (M = Ir, Rh) Superconductors: Insights from DFT-Based Computer Simulation. <b>2021</b> , 34, 1775-1789	1
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561	Structural, elastic, and electronic properties of MgB <sub>2</sub> C <sub>2</sub> under pressure from first-principles calculations. <b>2021</b> , 121, e26442	1
560	Effect of transition metal element additions on the mechanical and electronic properties of L10 CoNi alloys. <b>2021</b> , 42, 101128	1
559	Structural, mechanical, thermodynamic and electronic properties of Pt <sub>3</sub> M (M = Al, Co, Hf, Sc, Y, Zr) compounds under high pressure. <b>2021</b> , 40, 1208-1218	4
558	Dense as diamond: Pn-C <sub>10</sub> , a superhard sp <sup>3</sup> carbon allotrope. <b>2021</b> , 118, 012107	1
557	Elastic properties of superionic cubic silver sulfide $\beta$ -Ag <sub>2</sub> S. <b>2021</b> , 23, 2914-2922	5
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553	Elastic, mechanical, anisotropic, optical and magnetic properties of V <sub>2</sub> NiSb Heusler alloy. <b>2021</b> , 96, 035807	5
552	Elastic anisotropy of mechanically responsive molecular solids. <b>2021</b> , 23, 5805-5814	0
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550	A Theoretical Investigation on the Physical Properties of SrPd <sub>2</sub> Sb <sub>2</sub> Superconductor. <b>2021</b> , 34, 1133-1139	6

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546	Effect of nonstoichiometry on elastic properties of niobium carbide NbC. <b>2021</b> , 95, 105435	9
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544	Chiral triclinic metamaterial crystals supporting isotropic acoustical activity and isotropic chiral phonons. <b>2021</b> , 477, 20200764	4
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541	The thermodynamic stability and mechanical properties of TiC <sub>x</sub> N <sub>1-x</sub> (0 ≤ x ≤ 1) compounds by cluster expansion method and first-principles calculations. <b>2021</b> ,	
540	Structural, elastic and mechanical properties of Ti <sub>1-5</sub> Nb <sub>x</sub> Ge alloys: insight from DFT calculations. <b>2021</b> , 44, 1	3
539	Effect of alloying elements on the structure and mechanical properties of NbMoTaWX (X = Cr, V, Ti, Zr, and Hf) refractory high-entropy alloys. <b>2021</b> , 11, 025044	2
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537	Study on mechanical, electronic and optical properties of Pb-free double halide perovskites In <sub>2</sub> TiX <sub>6</sub> (X = Cl, Br, I) for solar cells based on first-principles. <b>2021</b> , 26, 102180	1
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