

Bi-Yu Tang

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	First-principles study of elastic and electronic properties of MgZn ₂ and ScZn ₂ phases in Mg ^{1-x} Sc ^x Zn alloy. Journal of Alloys and Compounds, 2010, 506, 412-417.	5.5	135
2	Elastic and thermodynamic properties of high entropy carbide (HfTaZrTi)C and (HfTaZrNb)C from ab initio investigation. Ceramics International, 2020, 46, 15104-15112.	4.8	58
3	Ab Initio Prediction of Mechanical and Electronic Properties of Ultrahigh Temperature High-Entropy Ceramics (Hf _{0.2} Zr _{0.2} Ta _{0.2} M _{0.2} Ti _{0.2})B ₂ (M = Nb, Mo, Cr). Physica Status Solidi (B): Basic Research, 2018, 255, 1800011.	1.5	48
4	Stability of MgO(111) Polar Surface: Effect of the Environment. Journal of Physical Chemistry C, 2008, 112, 3327-3333.	3.1	26
5	Mechanical properties of L1 ₂ type Al ₃ X (X = Mg, Sc, Zr) from first-principles study. Physica Status Solidi (B): Basic Research, 2012, 249, 1510-1516.	1.5	23
6	First-Principles Investigation of Dehydrogenation on Cu-Doped MgH ₂ (001) and (110) Surfaces. Journal of Physical Chemistry C, 2014, 118, 13607-13616.	3.1	23
7	First-principles study on the elastic properties of B ² and Q phase in Al ^{1-x} Mg ^x Si ^x (x = Cu) alloys. Physica Scripta, 2013, 87, 015601.	2.5	22
8	Electronic structure and Fermi surface character of LaNiPO from first principles. Physical Review B, 2008, 77, .	3.2	19
9	First-principles study of (Ti ^{1-x} Mg ^x)Si ₃ phases with the hexagonal D88 structure: Elastic properties and electronic structure. Computational Materials Science, 2012, 54, 287-292.	3.0	16
10	Ab initio study of I2 and T2 stacking faults in C14 Laves phase MgZn ₂ . European Physical Journal B, 2013, 86, 1.	1.5	16
11	First-principles study of point defects in C14 MgZn ₂ Laves phase. Journal of Alloys and Compounds, 2016, 654, 475-481.	5.5	16
12	Effects of Y and Zn atoms on the elastic properties of Mg solid solution from first-principles calculations. Physica Status Solidi (B): Basic Research, 2011, 248, 2809-2815.	1.5	12
13	Elastic and electronic properties of ScMn ₂ from first-principles calculations. Physica B: Condensed Matter, 2010, 405, 4812-4817.	2.7	10
14	Influence of Local Lattice Distortion on Elastic Properties of Hexagonal Close-Packed TiZrHf and TiZrHfSc Refractory Alloys. Physica Status Solidi (B): Basic Research, 2021, 258, 2100025.	1.5	10
15	Possible new metastable Mo ₂ Ga ₂ C and its phase transition under pressure: a density functional prediction. Journal of Materials Science, 2016, 51, 8452-8460.	3.7	8
16	Elastic properties and electronic structures of Mg _{1-x} Ce _x intermetallic compounds from first-principles calculations. Physica Status Solidi (B): Basic Research, 2011, 248, 2097-2102.	1.5	7
17	Elastic properties of random L1 ₂ Al ₃ (Sc _{0.5} TM _{0.5}) alloys from first-principle SQSs calculations. Journal of Materials Science, 2012, 47, 3793-3800.	3.7	7
18	Crystal feature and electronic structure of novel mixed alanate LiCa(AlH ₄) ₃ : a density functional theory investigation. RSC Advances, 2015, 5, 16439-16445.	3.6	6

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19	Mechanical behavior of high entropy carbide (HfTaZrTi)C and (HfTaZrNb)C under high pressure: Ab initio study. International Journal of Quantum Chemistry, 2021, 121, e26509.	2.0	6
20	ROTATIONAL ALIGNMENT OF PRODUCT MOLECULES FROM THE REACTION $\text{Ca} + \text{HCl} \rightarrow \text{CaCl} + \text{H}$. Journal of Theoretical and Computational Chemistry, 2011, 10, 19-29.	1.8	5
21	Correlation between mechanical properties and valence electron concentration for NbTiZrM ($\text{M} = \text{Hf}$), Tj ETQq1 1 0.784314 Processing, 2021, 127, 1.	2.3	5
22	First-Principle Calculations of the MgYA4 ($\text{A} = \text{Co}$ and Ni) Phase with AuBe5-Type Structure. Acta Metallurgica Sinica (English Letters), 2015, 28, 1326-1331.	2.9	4
23	Theoretical study of the CsMgH_3 , Cs_2MgH_4 and $\text{Cs}_4\text{Mg}_3\text{H}_{10}$ complex hydrides from first principles. Physica Status Solidi (B): Basic Research, 2008, 245, 2749-2755.	1.5	3
24	Intrinsic point defects in ternary MgCaSi: Ab initio investigation. Journal of Materials Research, 2017, 32, 3723-3731.	2.6	3
25	Temperature-dependent elastic properties of high entropy ceramic (ZrTaNbTi)C from self-consistent quasi-harmonic approximation. Solid State Communications, 2021, 336, 114432.	1.9	3
26	First-principles study on mechanical properties of LaMg_3 and LaCuMg_2 . Journal of Central South University, 2014, 21, 2136-2142.	3.0	2
27	Thermodynamic Properties of $\text{W}_x(\text{TaTiVCr})_{1-x}$ High-Entropy (Like) Alloy and Influence of Tungsten Content. Physica Status Solidi (B): Basic Research, 2019, 256, 1800741.	1.5	2
28	Structural and mechanical properties of ternary MgCaSi phase: A study by density functional theory. Journal of Chemical Research, 2020, 44, 50-59.	1.3	2
29	An initio study of influence of substitution of Sc with Al on intrinsic mechanical properties of hexagonal high-entropy alloys $\text{Hf}_{0.25}\text{Ti}_{0.25}\text{Zr}_{0.25}\text{Sc}_{0.25-x}\text{Al}_x$ ($x \leq 15\%$). Materials Today Communications, 2021, 29, 102875.	1.9	2
30	$\{110\}$ dislocation core properties in $\text{L1}_2\text{-Al}_3\text{Sc}$ and Al_3Mg based on the Peierls-Nabarro model. Physica Status Solidi (B): Basic Research, 2013, 250, 1825-1831.	1.5	1
31	Novel elastic evolution of carbide $\text{Mo}_2\text{Ga}_2\text{C}$ under pressure: Ab initio theoretical investigation. International Journal of Modern Physics B, 2019, 33, 1950358.	2.0	1
32	Stacking fault energy of basal plane for hexagonal closed-packed medium entropy alloy ZrHfTi : Ab initio prediction. Applied Physics A: Materials Science and Processing, 2021, 127, 1.	2.3	1