

Gboyega A Adebayo

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Effect of guest atoms on structural properties, electronics structure and optical spectra of $B_xCo_4-XSb_{12}$ ($X = 0$ or 1 , $B = Fe$ or Al) skutterudites. Materials Science in Semiconductor Processing, 2022, 139, 106340.	4.0	0
2	Electronic, Structural, Mechanical, and Thermodynamic Properties of $CoYSb$ ($Y = Cr, Mo, W$) Half-Heusler Compounds as Potential Spintronic Materials. Solids, 2022, 3, 22-33.	2.4	10
3	First principle calculations of the structural, elastic, electronic and transport properties of $XRuAs$ ($X = Ta$ and V). Materials Science in Semiconductor Processing, 2022, 148, 106837.	4.0	4
4	Predicting the band structure, transport properties, electronic fitness function and effective mass of $PdTiSn$ indirect band-gap half-Heusler semiconductor. Materials Science in Semiconductor Processing, 2021, 123, 105548.	4.0	4
5	Electronic fitness function, effective mass and thermoelectric properties of Rh-based (-ScTe; -TiSb;) $T_j ETQq1 1 0.784314 rgBT /Overclock$ e00523.	2.1	6
6	Band structure and absorption spectra of NH_4XI_3 ($X = Pb, Mg$) based hybrid Perovskite for UV ray protector and electrochromic materials applications. Journal of Physics and Chemistry of Solids, 2021, 151, 109860.	4.0	4
7	Exploring the electronic fitness function, effective mass, elastic and transport properties of $RhTiP$ Half-Heusler alloy. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2021, 264, 114987.	3.5	7
8	Thermoelectric and mechanical properties of $XHfSn$ ($X=Ni, Pd$ and Pt) semiconducting Half-heusler alloys: A first-principles study. Computational Condensed Matter, 2021, 26, e00539.	2.1	13
9	Investigation of the thermoelectric properties of Lithium-Aluminium-Silicide ($LiAlSi$) compound from first-principles calculations. Computational Condensed Matter, 2021, 27, e00551.	2.1	10
10	Assessing the structural, electronic, elastic and thermoelectric properties of $PtTiSn$ and $PdLaBi$ transition metal alloys from the first-principles prospective. Materials Science in Semiconductor Processing, 2021, 129, 105796.	4.0	3
11	The effective mass, fitness function and enhanced thermoelectric properties in $CuSbS_2$ for p-type thermoelectric material applications: Density functional theory approach. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2021, 273, 115404.	3.5	4
12	Skutterudite materials; $AlyFe_xCo_4-x-ySb_{12}$ ($x = y = 1$; $x = 2, y = 1$) for spintronics and optoelectronics applications. Computational Condensed Matter, 2021, 29, e00613.	2.1	0
13	Bandgap Correction and Spin-Orbit Coupling Induced Absorption Spectra of Dimethylammonium Lead Iodide for Solar Cell Absorber. Frontiers in Energy Research, 2021, 9, .	2.3	1
14	Unraveling the Stable Phase, High Absorption Coefficient, Optical and Mechanical Properties of Hybrid Perovskite $CH_3NH_3PbxMg_1-xI_3$: Density Functional Approach. Journal of Inorganic and Organometallic Polymers and Materials, 2020, 30, 299-309.	3.7	16
15	Band structure, thermoelectric properties, effective mass and electronic fitness function of two newly discovered 18 valence electrons stable half-Heusler TaX ($X=Co,Ir$) Sn semiconductors: A density functional theory approach. Solid State Sciences, 2020, 100, 106096.	3.2	4
16	Lattice dynamics and thermodynamic investigation of $MNiSn$ ($M=\text{Hf, Ti and Zr}$) Half-Heusler compounds: Density functional theory approach. Materials Today Communications, 2020, 22, 100671.	1.9	5
17	Design and theoretical study of phenothiazine-based low bandgap dye derivatives as sensitizers in molecular photovoltaics. Optical and Quantum Electronics, 2020, 52, 1.	3.3	16
18	Structural evolution, electronic and physicochemical properties of tin ozonide nanoclusters: a density functional theory perspective. Journal of Nanoparticle Research, 2020, 22, 1.	1.9	0

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19	First-principles perspective on structural evolution, sequential lithiation and physicochemical properties of tin oxide nanoclusters: Sn_3O_2 and $\text{Li}_x\text{Sn}_3\text{O}_2$ ($x = 1-10$ and $z = 0, 3-7$). Materials Today Communications, 2020, 24, 101026.	1.9	0
20	Predicting the stable Type-I phase of $\text{X}_2\text{M}_2\text{O}_6$ ($\text{X} = \text{Co}, \text{Fe}, \text{Os}$) compounds and its thermodynamic, electronic and magnetic properties from first-principles calculations. Solid State Sciences, 2020, 105, 106208.	3.2	6
21	DFT GGA calculations of magnetic, elastic, thermodynamic and thermoelectric properties of Co_2YAl ($\text{Y} = \text{Ti}, \text{V}$) full Heusler alloy systems. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2020, 262, 114739.	3.5	11
22	Thermoelectric properties, optimal doping levels and high figure of merit in Cobalt-based Half/Full Heusler alloys by First-Principles calculations. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2019, 248, 114409.	3.5	3
23	Predicting the elastic, phonon and thermodynamic properties of cubic HfNiX ($X = \text{Ge}$ and Sn) Half Heusler alloys: a DFT study. European Physical Journal B, 2019, 92, 1.	1.5	11
24	A density functional theory analysis of the mechanical and dynamic stability and thermodynamic properties of pyrite-type ZnSe_2 and ZnTe_2 . Computational Condensed Matter, 2019, 19, e00366.	2.1	0
25	Effects of Y atom substitution on the structural, magnetic, electronic, elastic, mechanical, thermodynamic and thermoelectric properties of Co_2YAl ($\text{Y} = \text{Cr}, \text{Mn}$) Full Heusler alloys from first principles investigations. Computational Condensed Matter, 2019, 21, e00412.	2.1	14
26	First principles comparative studies of thermoelectric and other properties in the cubic and hexagonal structure of CsCdCl_3 halide perovskites. Computational Condensed Matter, 2019, 21, e00388.	2.1	8
27	First principle calculations of structural, electronic, optical and thermoelectric properties of tin (II) oxide. Materials Research Express, 2019, 6, 125915.	1.6	9
28	DFT investigation of elastic, mechanical, vibrational and thermodynamic properties of cadmium dichalcogenides. Physica B: Condensed Matter, 2019, 552, 159-164.	2.7	7
29	CK-RAID: Collaborative Knowledge Repository for Intrusion Detection System. Journal of Computing and Information Technology, 2019, 27, 29-39.	0.3	0
30	First-principles calculations of dynamical and thermodynamic properties of cuprite doped with silver ($\text{Cu}_2(1-x)\text{Ag}_x\text{O}$). Materials Research Express, 2018, 5, 045704.	1.6	5
31	First-principle survey of structural, electronic, and optical properties of zinc blende $\text{Al}_2\text{Ga}_x\text{Ga}_{2-x}\text{As}$. Materials Letters, 2018, 221, 330-335.	2.6	2
32	Increased Malleability in Tetragonal $\text{Zr}_x\text{Ti}_{1-x}\text{O}_2$ Ternary Alloys: First-Principles Approach. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2017, 72, 567-572.	1.5	1
33	Elastic constants and observed ferromagnetism in inverse Heusler alloy Ti_2CoAs using kpw pseudopotentials: A first-principles approach. Journal of Alloys and Compounds, 2017, 722, 207-211.	5.5	10
34	Elastic constants and mechanical properties of PEDOT from first principles calculations. Computational Materials Science, 2017, 139, 234-242.	3.0	15
35	Ab initio study of phonon dispersion and thermodynamic properties of pure and doped pyrites. European Physical Journal B, 2017, 90, 1.	1.5	7
36	Structural, Electronic, Magnetic and Optical Properties of Ni,Ti/Al-based Heusler Alloys: A First-Principles Approach. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2016, 71, 129-134.	1.5	7

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37	First-principles study of zinc-blende $B_xAl_{yIn_{1-x-y}}N$ quaternary alloy: Alchemical mixing approximation approach. International Journal of Modern Physics B, 2016, 30, 1650191.	2.0	1
38	Prediction of metallic and half-metallic structure and elastic properties of $\text{Fe}_{x}\text{Ti}_{1-x}$. International Journal of Modern Physics B, 2013, 27, 1471-1477.	2.0	1
39	First principles study of electronic structure, structural and optical properties of $\text{Mg}_3\text{Si}_2\text{O}_5(\text{OH})_4$. Applied Clay Science, 2014, 93-94, 8-11.	5.2	6
40	Structural and elastic properties of strained $\text{Mg}_{1-x}\text{Sr}_x\text{Se}$ revealed. Solid State Communications, 2014, 178, 46-49.	1.9	1
41	Analysis and interpretation of Ibuji spring magnetic anomaly using the Mellin transform. Open Geosciences, 2013, 5, .	1.7	1
42	Ab initio calculations of optical properties of Li and K at high pressures. Journal of Physics and Chemistry of Solids, 2013, 74, 1221-1226.	4.0	2
43	ELECTRONIC AND ELASTIC PROPERTIES OF ZINC-BLENDE MgSe . International Journal of Modern Physics B, 2013, 27, 1350027.	2.0	5
44	First principles studies of band structure and electronic properties of ZnSe . Journal of Alloys and Compounds, 2012, 513, 294-299.	5.5	20
45	ANTISYNCHRONIZATION OF IDENTICAL AND NONIDENTICAL \dot{x}^1 VAN DER POL AND \dot{x}^2 DUFFING OSCILLATORS WITH BOTH PARAMETRIC AND EXTERNAL EXCITATIONS VIA BACKSTEPPING APPROACH. International Journal of Modern Physics B, 2011, 25, 1957-1969.	2.0	3
46	Adhesion energy, surface traction and surface tension in liquid xenon. Pramana - Journal of Physics, 2011, 77, 1151-1157.	1.8	1
47	Optical properties of revealed by ab initio calculations. Journal of Physics and Chemistry of Solids, 2010, 71, 1690-1693.	4.0	5
48	Collision frequency of Lennard-Jones fluids at high densities by equilibrium molecular dynamics simulation. Pramana - Journal of Physics, 2010, 75, 523-536.	1.8	5
49	Electronic structure and optical properties of from ab initio calculations. Physica B: Condensed Matter, 2010, 405, 4578-4581.	2.7	6
50	Generalized control and synchronization of chaos in RCL-shunted Josephson junction using backstepping design. Physica C: Superconductivity and Its Applications, 2010, 470, 558-564.	1.2	45
51	Mixing properties in the $\text{In}-\text{Pb}$ and $\text{In}-\text{Mg}$ liquid alloys. Physica B: Condensed Matter, 2010, 405, 880-887.	2.7	3
52	Infrared absorption of MgO at high pressures and temperatures: A molecular dynamic study. Journal of Chemical Physics, 2009, 131, 014506.	3.0	15
53	Thermodynamics and surface properties of liquid $\text{Al}-\text{Ga}$ and $\text{Al}-\text{Ge}$ alloys. Applied Physics A: Materials Science and Processing, 2009, 97, 533-541.	2.3	16
54	Adhesion Energy, Surface Traction and Surface Tension in Fe-Mg Binary Alloys. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2007, 62, 596-600.	1.5	1

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55	Correlation between bulk and surface properties in Rb–Pb liquid alloy. <i>Journal of Molecular Liquids</i> , 2006, 128, 90-95.	4.9	1
56	Dynamical properties of Ag-Cu binary alloy from molecular dynamics simulation. <i>European Physical Journal B</i> , 2006, 54, 423-427.	1.5	2
57	Structures and autocorrelation functions of liquid Al and Mg modelled via Lennard-Jones potential from molecular dynamics simulation. <i>Pramana - Journal of Physics</i> , 2005, 64, 269-279.	1.8	7
58	Structural properties of low-density liquid alkali metals. <i>Pramana - Journal of Physics</i> , 2005, 65, 1085-1096.	1.8	3
59	Structure, single-particle and many-particle coefficients of Lennard-Jones liquid Al. <i>Pramana - Journal of Physics</i> , 2005, 65, 339-347.	1.8	0
60	Influence of strong heterocoordination on surface properties of Li–Pb melts. <i>Physics and Chemistry of Liquids</i> , 2005, 43, 495-506.	1.2	4
61	Quasi-chemical studies of ordering in the Cu-Zr and Cu-Si melts. <i>Journal of Alloys and Compounds</i> , 2001, 329, 162-167.	5.5	11
62	Structural properties of undercooled liquid sodium and caesium. <i>Pramana - Journal of Physics</i> , 1999, 52, 631-645.	1.8	2