Habib Rached

List of Publications by Year
in descending order

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65 papers	1,566 citations	331259 21 h-index	360668 35 g-index
65 all docs	65 docs citations	65 times ranked	712 citing authors

#	Article	IF	Citations
1	Structural, mechanical, electronic and magnetic properties of a new series of quaternary Heusler alloys CoFeMnZ (Z=Si, As, Sb): A first-principle study. Journal of Magnetism and Magnetic Materials, 2015, 393, 165-174.	1.0	109
2	Electronic structure and magnetic properties of quaternary Heusler alloys CoRhMnZ (ZÂ=ÂAl, Ga, Ge) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	2.8	101
3	Firstâ€principles calculations of structural, elastic and electronic properties of Ni₂MnZ (Z) Tj ETQq1 1 0.784314 rgBT /Ov	0.7	86
4	Investigation of Iron-based double perovskite oxides on the magnetic phase stability, mechanical, electronic and optical properties via first-principles calculation. Materials Chemistry and Physics, 2017, 193, 453-469.	2.0	68
5	Full-potential calculation of the structural, elastic, electronic and magnetic properties of XFeO3 (X=Sr and Ba) perovskite. Physica B: Condensed Matter, 2010, 405, 3515-3519.	1.3	64
6	Computational study of structural, elastic and electronic properties of lithium disilicate (Li 2 Si 2 O 5) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.5	52
7	First-principles investigations of Na2CuMCl6 (M = Bi, Sb) double perovskite semiconductors: Materials for green technology. Materials Science in Semiconductor Processing, 2022, 150, 106947.	1.9	45
8	The half metallic feature at high temperature of the novel half-Heusler alloys and their [100] oriented layered superlattices: A DFT investigations. Materials Chemistry and Physics, 2021, 267, 124712.	2.0	43
9	Pressure effects on the structural, elastic, magnetic and thermodynamic properties of Mn2AlC and Mn2SiC MAX phases. Journal of Alloys and Compounds, 2021, 885, 160998.	2.8	40
10	Theoretical Insight into the Stability, Magneto-electronic and Thermoelectric Properties of XCrSb (X:) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 2022, 35, 875-887.	0.8	40
11	Theoretical investigation of the structural, electronic, magnetic and elastic properties of binary cubic C15-Laves phases TbX2 (XÂ=ÂCo and Fe). Journal of Alloys and Compounds, 2016, 689, 885-893.	2.8	38
12	Study of the structural, mechanical and thermodynamic properties of the new MAX phase compounds (Zr1-xTix)3AlC2. Computational Condensed Matter, 2020, 23, e00468.	0.9	37
13	A first principle study of phase stability, electronic structure and magnetic properties for Co2â^'xCrxMnAl Heusler alloys. Journal of Magnetism and Magnetic Materials, 2015, 379, 84-89.	1.0	36
14	Investigation of electronic structure, magnetic properties and thermal properties of the new half-metallic ferromagnetic full-Heusler alloys Cr2GdSi1â^'xGex: An ab-initio study. Journal of Alloys and Compounds, 2016, 676, 440-451.	2.8	34
15	First-principles study of structural stabilities, elastic and electronic properties of transition metal monocarbides (TMCs) and mononitrides (TMNs). Materials Chemistry and Physics, 2013, 143, 93-108.	2.0	33
16	A comprehensive computational investigations on the physical properties of <scp>TiXSb</scp> (X: Ru,) Tj ETQq0 0 0 rgBT /Overlock 10 <scp>halfâ€Heusler</scp>. International Journal of Quantum Chemistry, 2022, 122, .	1.0	33
17	A Comparative Study of Structural Stability and Mechanical and Optical Properties of Fluorapatite (Ca5(PO4)3F) and Lithium Disilicate (Li2Si2O5) Components Forming Dental Glassâ€“Ceramics: First Principles Study. Journal of Electronic Materials, 2016, 45, 5082-5095.	1.0	32
18	DFT study with different exchange-correlation potentials of physical properties of the new synthesized alkali-metal based Heusler alloy. European Physical Journal B, 2020, 93, 1.	0.6	32

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19	Firstâ€principles calculations to investigate structural stabilities, mechanical and optoelectronic properties of <scp>NbCoSn</scp> and <scp>NbFeSb halfâ€Heusler</scp> compounds. International Journal of Quantum Chemistry, 2021, 121, e26582.	1.0	32
20	Structural, electronic and mechanical properties of RuO2 from first-principles calculations. Materials Science in Semiconductor Processing, 2012, 15, 331-339.	1.9	25
21	Structural stability, electronic structure and magnetic properties of the new hypothetical half-metallic ferromagnetic full-Heusler alloy CoNiMnSi. Materials Science-Poland, 2016, 34, 85-93.	0.4	25
22	Spin Gapless Semiconductor Behavior in d^{â˜}-d Half-Heusler CrSbSr: Potential Candidate for Spintronic Application. Spin, 2020, 10, .	0.6	24
23	The half metallic behavior at high temperature of highly spin-polarized V-based Heusler alloy: DFT calculations. European Physical Journal B, 2021, 94, 1.	0.6	22
24	Theoretical investigation of magnetic, electronic, thermoelectric and thermodynamic properties of Fe2TaZ (Z= B, In) compounds by GGA and GGA+U approaches. Computational Condensed Matter, 2020, 22, e00438.	0.9	21
25	The Vanadium-doping effect on physical properties of the Zr2AlC MAX phase compound. Materials Chemistry and Physics, 2021, 260, 124189.	2.0	21
26	Prediction of stabilities phase and elastic properties of Palladium Carbide. Computational Materials Science, 2010, 48, 556-562.	1.4	20
27	Prediction of a new quaternary Heusler alloy within a good electrical response at high temperature for spintronics applications: <scp>DFT</scp> calculations. International Journal of Quantum Chemistry, 2021, 121, e26647.	1.0	20
28	Prediction study of the structural, elastic, electronic and optical properties of the antiperovskite. Solid State Communications, 2009, 149, 2002-2006.	0.9	19
29	Ab Initio Study of Electronic Structure, Elastic and Transport Properties of Fluoroperovskite LiBeF3. Journal of Electronic Materials, 2017, 46, 2205-2210.	1.0	19
30	Magneto-electronic, mechanical and thermodynamic properties of full-Heusler alloys Cr2GdGe1-xSnx. Journal of Alloys and Compounds, 2018, 742, 736-750.	2.8	19
31	The stability analysis and efficiency of the new MAX-phase compounds M3GaC2 (M: Ti or Zr): A first-principles assessment. Results in Physics, 2022, 38, 105621.	2.0	19
32	Ab-initio prediction of high TC half-metallic ferrimagnetism in Li-based Heusler compounds Mn2LiZ (ZÂ=) Tj ETQq0 0 0 rgBT /Overlock 10	0.9	18
33	Full potential calculation of structural, elastic properties and high-pressure phase of binary noble metal carbide: ruthenium carbide. Journal of Physics and Chemistry of Solids, 2010, 71, 1780-1784.	1.9	17
34	Insight into the structural, electronic, mechanical and optical properties of inorganic lead bromide perovskite APbBr3 (AÂ= Li, Na, K, Rb, and Cs). Computational Condensed Matter, 2020, 24, e00478.	0.9	17
35	First-Principle Study of Half-Metallic Ferrimagnet Behavior in Titanium-Based Heusler Alloys Ti2FeZ (Z) Tj ETQq1 1 0.784314 rgBT /Ove	0.8	16
36	Investigation of Structural, Elastic, Electronic, Magnetic and Thermoelectric Proprieties for Mn2RhZ (Zâ€‰=â€‰Al, Si and Ge) Full-Heusler Alloys. International Journal of Thermophysics, 2021, 42, 1.	1.0	16

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37	DFT calculations of structural, optoelectronic and thermodynamic properties of BxAl1-xP alloys. Computational Condensed Matter, 2019, 19, e00377.	0.9	15
38	Theoretical Studies of the Structural, Electronic and Magnetic Properties of the CoFeCeZ (Z = P, As) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	0.6	15
39	Electronic structure and optoelectronic behavior of MgPbP2 chalcopyrite. Computational Condensed Matter, 2021, 27, e00550.	0.9	15
40	Prediction of double transition metal (<scp>Cr_{1â^'x}Zr_x</scp>)<scp>₂AlC MAX</scp> phases as thermal barrier coatings: Insight from density functional theory. International Journal of Quantum Chemistry, 2021, 121, e26770.	1.0	15
41	Investigation of Ruthenium based Full-Heusler compound for thermic, spintronics and thermoelectric applications: DFT computation. Materials Science in Semiconductor Processing, 2021, 134, 106047.	1.9	15
42	Computational determination of structural, electronic, magnetic and thermodynamic properties of Co2HfZ (ZÂ=ÂAl, Ga, Si and Sn) full Heusler compounds for spintronic applications. Journal of Alloys and Compounds, 2022, 894, 162503.	2.8	15
43	The Structural, Electronic, Optical and Thermo-Electric Properties of Oxynitride Perovskite CaTaO₂N. Spin, 2020, 10, .	0.6	14
44	Spin gapless semiconductor and nearly spin semimetal antiferromagnets: The case of the inverse Heusler compounds Mn2LiZ (ZÂ=ÂAl and Ga). Materials Research Bulletin, 2021, 143, 111461.	2.7	14
45	Full potential study of the structural, electronic and optical properties of (InAs)m/(GaSb)n superlattices. Computational Condensed Matter, 2019, 21, e00394.	0.9	13
46	The Stability and Electronic and Thermal Transport Properties of New Tlâ€Based MAXâ€Phase Compound Ta₂TlX (X: C or N). Physica Status Solidi (B): Basic Research, 2022, 259, .	0.7	13
47	A Theoretical Analysis of Physical Properties and Half-Metallic Stability under Pressure Effect of the ScNiCrZ (Z=Ga, Al, In) Heusler Alloys. Spin, 2021, 11, .	0.6	12
48	Prediction of a new Sn-based MAX phases for nuclear industry applications: DFT calculations. Materials Today Communications, 2021, 27, 102233.	0.9	12
49	Magneto-electronic and thermoelectric properties of V-based Heusler in ferrimagnetic phase. Applied Physics A: Materials Science and Processing, 2022, 128, .	1.1	12
50	Study of structural, elastic and electronic properties of GdX (X=Bi, Sb) compounds using LSDA and LSDA+U approach. Computational Materials Science, 2011, 50, 1965-1972.	1.4	10
51	First-principles calculations of the elastic, and electronic properties of YFe2, NiFe2 and YNiFe4 intermetallic compounds. Computational Materials Science, 2013, 73, 56-64.	1.4	10
52	Electronic structure and optical properties of (BeTe)_n/(ZnSe)_m superlattices. Materials Science-Poland, 2016, 34, 115-125.	0.4	9
53	Prediction of phase transition, mechanical and electronic properties of inverse Heusler compound Y₂RuPb, via FP-LMTO method. International Journal of Modern Physics C, 2016, 27, 1650107.	0.8	9
54	Theoretical insight of stabilities and optoelectronic features of Ru-based Heusler alloys: Ab-initio calculations. Computational Condensed Matter, 2021, 28, e00573.	0.9	9

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55	Elastic stability, electronic structure and optical properties of PtN2 with pyrite and fluorite structures. Journal of Alloys and Compounds, 2009, 478, 297-302.	2.8	7
56	Structural stabilities, elastic, and electronic properties of iridium mononitride: a first-principles study. Phase Transitions, 2011, 84, 269-283.	0.6	7
57	Electronic structure, magnetic and structural properties of binary cubic C15 Laves phases PrX2 (Xâ€‰=â€‰Co) Tj ETQq1 1 0.78431	1.1	7
58	High-throughput study of the structural, electronic, and optical properties of short-period (BeSe)m/(ZnSe)n superlattices based on DFT calculations. Computational Condensed Matter, 2021, 29, e00598.	0.9	6
59	Electronic, optical, magnetic and thermoelectric properties of CsNiO$$_{mathrm {mathbf {2}}}$$ and CsCuO$$_{mathrm {2}}$$: Insights from DFT-based computer simulation. Pramana - Journal of Physics, 2021, 95, 1.	0.9	5
60	An extensive computational report on the quinary alloys Cu2Zn1â^'xCdxSnS4 for the solar cell systems: DFT simulation. Computational Condensed Matter, 2022, 31, e00670.	0.9	5
61	Theoretical investigation on the optoelectronic properties of ZrxSi1-xO2 tetragonal hypothetical alloys from zircon family. Applied Physics A: Materials Science and Processing, 2022, 128, 1.	1.1	4
62	Density functional theory study on the magneto-electronic, mechanical, thermal, and transport properties of a novel Co2VGa0.5Al0.5 quaternary Heusler alloy. Emergent Materials, 2022, 5, 1819-1830.	3.2	4
63	Elastic and electronic properties calculations of the filled skutterudite CeOs₄P₁₂. Journal of Physics: Conference Series, 2016, 758, 012010.	0.3	3
64	The effect of Lanthanide doping on the structural, elastic, thermodynamic and electronic properties of YBi: An ab-initio study. Computational Condensed Matter, 2018, 16, e00295.	0.9	3
65	Electronic structure of short-period ZnSe/ZnTe superlattices based on DFT calculations. Condensed Matter Physics, 2022, 25, 13701.	0.3	1