

# Habib Rached

## List of Publications by Citations

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60  
papers

753  
citations

15  
h-index

25  
g-index

65  
ext. papers

1,080  
ext. citations

2.6  
avg, IF

4.58  
L-index

#	Paper	IF	Citations
60	Structural, mechanical, electronic and magnetic properties of a new series of quaternary Heusler alloys CoFeMnZ (Z=Si, As, Sb): A first-principle study. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2015</b> , 393, 165-174	2.8	83
59	Electronic structure and magnetic properties of quaternary Heusler alloys CoRhMnZ (Z=Al, Ga, Ge and Si) via first-principle calculations. <i>Journal of Alloys and Compounds</i> , <b>2015</b> , 647, 276-286	5.7	73
58	First-principles calculations of structural, elastic and electronic properties of Ni <sub>2</sub> MnZ (Z = Al, Ga and In) Heusler alloys. <i>Physica Status Solidi (B): Basic Research</i> , <b>2009</b> , 246, 1580-1586	1.3	59
57	Full-potential calculation of the structural, elastic, electronic and magnetic properties of XFeO <sub>3</sub> (X=Sr and Ba) perovskite. <i>Physica B: Condensed Matter</i> , <b>2010</b> , 405, 3515-3519	2.8	43
56	Investigation of Iron-based double perovskite oxides on the magnetic phase stability, mechanical, electronic and optical properties via first-principles calculation. <i>Materials Chemistry and Physics</i> , <b>2017</b> , 193, 453-469	4.4	37
55	Computational study of structural, elastic and electronic properties of lithium disilicate (Li <sub>2</sub> Si <sub>2</sub> O <sub>5</sub> ) glass-ceramic. <i>Journal of the Mechanical Behavior of Biomedical Materials</i> , <b>2014</b> , 32, 345-350	4.1	33
54	A Comparative Study of Structural Stability and Mechanical and Optical Properties of Fluorapatite (Ca <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> F) and Lithium Disilicate (Li <sub>2</sub> Si <sub>2</sub> O <sub>5</sub> ) Components Forming Dental Glass-Ceramics: First Principles Study. <i>Journal of Electronic Materials</i> , <b>2016</b> , 45, 5082-5095	1.9	23
53	Theoretical investigation of the structural, electronic, magnetic and elastic properties of binary cubic C15-Laves phases TbX <sub>2</sub> (X = Co and Fe). <i>Journal of Alloys and Compounds</i> , <b>2016</b> , 689, 885-893	5.7	23
52	A first principle study of phase stability, electronic structure and magnetic properties for Co <sub>2</sub> CrxMnAl Heusler alloys. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2015</b> , 379, 84-89	2.8	22
51	Investigation of electronic structure, magnetic properties and thermal properties of the new half-metallic ferromagnetic full-Heusler alloys Cr <sub>2</sub> GdSi <sub>1-x</sub> Gex: An ab-initio study. <i>Journal of Alloys and Compounds</i> , <b>2016</b> , 676, 440-451	5.7	22
50	First-principles study of structural stabilities, elastic and electronic properties of transition metal monocarbides (TMCs) and mononitrides (TMNs). <i>Materials Chemistry and Physics</i> , <b>2013</b> , 143, 93-108	4.4	20
49	Structural stability, electronic structure and magnetic properties of the new hypothetical half-metallic ferromagnetic full-Heusler alloy CoNiMnSi. <i>Materials Science-Poland</i> , <b>2016</b> , 34, 85-93	0.6	18
48	Study of the structural, mechanical and thermodynamic properties of the new MAX phase compounds (Zr <sub>1-x</sub> Tix) <sub>3</sub> AlC <sub>2</sub> . <i>Computational Condensed Matter</i> , <b>2020</b> , 23, e00468	1.7	18
47	Structural, electronic and mechanical properties of RuO <sub>2</sub> from first-principles calculations. <i>Materials Science in Semiconductor Processing</i> , <b>2012</b> , 15, 331-339	4.3	16
46	Prediction study of the structural, elastic, electronic and optical properties of the antiperovskite BiNBa <sub>3</sub> . <i>Solid State Communications</i> , <b>2009</b> , 149, 2002-2006	1.6	15
45	Prediction of stabilities phase and elastic properties of Palladium Carbide. <i>Computational Materials Science</i> , <b>2010</b> , 48, 556-562	3.2	14
44	DFT study with different exchange-correlation potentials of physical properties of the new synthesized alkali-metal based Heusler alloy. <i>European Physical Journal B</i> , <b>2020</b> , 93, 1	1.2	14

43	Ab Initio Study of Electronic Structure, Elastic and Transport Properties of Fluoroperovskite LiBeF <sub>3</sub> . <i>Journal of Electronic Materials</i> , <b>2017</b> , 46, 2205-2210	1.9	13
42	Full potential calculation of structural, elastic properties and high-pressure phase of binary noble metal carbide: ruthenium carbide. <i>Journal of Physics and Chemistry of Solids</i> , <b>2010</b> , 71, 1780-1784	3.9	13
41	Magneto-electronic, mechanical and thermodynamic properties of full-Heusler alloys Cr <sub>2</sub> GdGe <sub>1-x</sub> Sn <sub>x</sub> . <i>Journal of Alloys and Compounds</i> , <b>2018</b> , 742, 736-750	5.7	12
40	Theoretical investigation of magnetic, electronic, thermoelectric and thermodynamic properties of Fe <sub>2</sub> TaZ (Z= B, In) compounds by GGA and GGA+U approaches. <i>Computational Condensed Matter</i> , <b>2020</b> , 22, e00438	1.7	12
39	First-Principle Study of Half-Metallic Ferrimagnet Behavior in Titanium-Based Heusler Alloys Ti <sub>2</sub> FeZ (Z = Al, Ga, and In). <i>Journal of Superconductivity and Novel Magnetism</i> , <b>2018</b> , 31, 1059-1065	1.5	11
38	Pressure effects on the structural, elastic, magnetic and thermodynamic properties of Mn <sub>2</sub> AlC and Mn <sub>2</sub> SiC MAX phases. <i>Journal of Alloys and Compounds</i> , <b>2021</b> , 885, 160998	5.7	11
37	Spin Gapless Semiconductor Behavior in d <sup>7</sup> -d Half-Heusler CrSbSr: Potential Candidate for Spintronic Application. <i>Spin</i> , <b>2020</b> , 10, 2050025	1.3	10
36	First-principles calculations to investigate structural stabilities, mechanical and optoelectronic properties of NbCoSn and NbFeSb half-Heusler compounds. <i>International Journal of Quantum Chemistry</i> , <b>2021</b> , 121, e26582	2.1	10
35	Study of structural, elastic and electronic properties of GdX (X = Bi, Sb) compounds using LSDA and LSDA + U approach. <i>Computational Materials Science</i> , <b>2011</b> , 50, 1965-1972	3.2	9
34	Theoretical Studies of the Structural, Electronic and Magnetic Properties of the CoFeCeZ (Z = P, As and Sb) Quaternary Heusler Alloys. <i>Spin</i> , <b>2020</b> , 10, 2050002	1.3	9
33	First-principles calculations of the elastic, and electronic properties of YFe <sub>2</sub> , NiFe <sub>2</sub> and YNiFe <sub>4</sub> intermetallic compounds. <i>Computational Materials Science</i> , <b>2013</b> , 73, 56-64	3.2	8
32	Ab-initio prediction of high TC half-metallic ferrimagnetism in Li-based Heusler compounds Mn <sub>2</sub> LiZ (Z= Si, Ge and Sn). <i>Computational Condensed Matter</i> , <b>2021</b> , 27, e00557	1.7	7
31	Electronic structure and optical properties of (BeTe) <sub>n</sub> /(ZnSe) <sub>m</sub> superlattices. <i>Materials Science-Poland</i> , <b>2016</b> , 34, 115-125	0.6	7
30	The half metallic feature at high temperature of the novel half-Heusler alloys and their [100] oriented layered superlattices: A DFT investigations. <i>Materials Chemistry and Physics</i> , <b>2021</b> , 267, 124712	4.4	7
29	The Structural, Electronic, Optical and Thermo-Electric Properties of Oxynitride Perovskite CaTaO <sub>2</sub> N. <i>Spin</i> , <b>2020</b> , 10, 2050007	1.3	6
28	Elastic stability, electronic structure and optical properties of PtN <sub>2</sub> with pyrite and fluorite structures. <i>Journal of Alloys and Compounds</i> , <b>2009</b> , 478, 297-302	5.7	6
27	The Vanadium-doping effect on physical properties of the Zr <sub>2</sub> AlC MAX phase compound. <i>Materials Chemistry and Physics</i> , <b>2021</b> , 260, 124189	4.4	6
26	Full potential study of the structural, electronic and optical properties of (InAs) <sub>m</sub> /(GaSb) <sub>n</sub> superlattices. <i>Computational Condensed Matter</i> , <b>2019</b> , 21, e00394	1.7	5

25	Prediction of phase transition, mechanical and electronic properties of inverse Heusler compound Y <sub>2</sub> RuPb, via FP-LMTO method. <i>International Journal of Modern Physics C</i> , <b>2016</b> , 27, 1650107	1.1	5
24	Structural stabilities, elastic, and electronic properties of iridium mononitride: a first-principles study. <i>Phase Transitions</i> , <b>2011</b> , 84, 269-283	1.3	5
23	Prediction of a new quaternary Heusler alloy within a good electrical response at high temperature for spintronics applications: DFT calculations. <i>International Journal of Quantum Chemistry</i> , <b>2021</b> , 121, e26647	2.1	5
22	DFT calculations of structural, optoelectronic and thermodynamic properties of B <sub>x</sub> Al <sub>1-x</sub> P alloys. <i>Computational Condensed Matter</i> , <b>2019</b> , 19, e00377	1.7	5
21	Investigation of Ruthenium based Full-Heusler compound for thermic, spintronics and thermoelectric applications: DFT computation. <i>Materials Science in Semiconductor Processing</i> , <b>2021</b> , 134, 106047	4.3	5
20	Insight into the structural, electronic, mechanical and optical properties of inorganic lead bromide perovskite APbBr <sub>3</sub> (A = Li, Na, K, Rb, and Cs). <i>Computational Condensed Matter</i> , <b>2020</b> , 24, e00478	1.7	4
19	A Theoretical Analysis of Physical Properties and Half-Metallic Stability under Pressure Effect of the ScNiCrZ (Z=Ga, Al, In) Heusler Alloys. <i>Spin</i> , <b>2021</b> , 11, 2150007	1.3	4
18	Computational determination of structural, electronic, magnetic and thermodynamic properties of Co <sub>2</sub> HfZ (Z = Al, Ga, Si and Sn) full Heusler compounds for spintronic applications. <i>Journal of Alloys and Compounds</i> , <b>2021</b> , 894, 162503	5.7	3
17	Investigation of Structural, Elastic, Electronic, Magnetic and Thermoelectric Properties for Mn <sub>2</sub> RhZ (Z = Al, Si and Ge) Full-Heusler Alloys. <i>International Journal of Thermophysics</i> , <b>2021</b> , 42, 1	2.1	3
16	Prediction of a new Sn-based MAX phases for nuclear industry applications: DFT calculations. <i>Materials Today Communications</i> , <b>2021</b> , 27, 102233	2.5	3
15	Prediction of double transition metal (Cr <sub>1-x</sub> Zr <sub>x</sub> ) <sub>2</sub> AlC MAX phases as thermal barrier coatings: Insight from density functional theory. <i>International Journal of Quantum Chemistry</i> , <b>2021</b> , 121, e26770	2.1	3
14	Elastic and electronic properties calculations of the filled skutterudite CeOs <sub>4</sub> P <sub>12</sub> . <i>Journal of Physics: Conference Series</i> , <b>2016</b> , 758, 012010	0.3	2
13	Spin gapless semiconductor and nearly spin semimetal antiferromagnets: The case of the inverse Heusler compounds Mn <sub>2</sub> LiZ (Z = Al and Ga). <i>Materials Research Bulletin</i> , <b>2021</b> , 143, 111461	5.1	2
12	The effect of Lanthanide doping on the structural, elastic, thermodynamic and electronic properties of YBi: An ab-initio study. <i>Computational Condensed Matter</i> , <b>2018</b> , 16, e00295	1.7	1
11	Theoretical Insight into the Stability, Magneto-electronic and Thermoelectric Properties of XCrSb (X: Fe, Ni) Half-Heusler Alloys and Their Superlattices. <i>Journal of Superconductivity and Novel Magnetism</i> , <b>2022</b> , 35, 875	1.5	1
10	Electronic, optical, magnetic and thermoelectric properties of CsNiO <sub>2</sub> and CsCuO <sub>2</sub> : Insights from DFT-based computer simulation <b>2021</b> , 95, 1		1
9	The half metallic behavior at high temperature of highly spin-polarized V-based Heusler alloy: DFT calculations. <i>European Physical Journal B</i> , <b>2021</b> , 94, 1	1.2	1
8	Electronic structure and optoelectronic behavior of MgPbP <sub>2</sub> chalcopyrite. <i>Computational Condensed Matter</i> , <b>2021</b> , 27, e00550	1.7	1

7	Theoretical insight of stabilities and optoelectronic features of Ru-based Heusler alloys: Ab-initio calculations. <i>Computational Condensed Matter</i> , <b>2021</b> , 28, e00573	1.7	1
6	The stability analysis and efficiency of the new MAX-phase compounds M <sub>3</sub> GaC <sub>2</sub> (M: Ti or Zr): A first-principles assessment. <i>Results in Physics</i> , <b>2022</b> , 38, 105621	3.7	1
5	Electronic structure, magnetic and structural properties of binary cubic C15 Laves phases PrX <sub>2</sub> (X = Co and Fe): a first-principles study. <i>Applied Physics A: Materials Science and Processing</i> , <b>2021</b> , 127, 1	2.6	0
4	High-throughput study of the structural, electronic, and optical properties of short-period (BeSe) <sub>m</sub> /(ZnSe) <sub>n</sub> superlattices based on DFT calculations. <i>Computational Condensed Matter</i> , <b>2021</b> , 29, e00598	1.7	0
3	Theoretical investigation on the optoelectronic properties of Zr <sub>x</sub> Si <sub>1-x</sub> O <sub>2</sub> tetragonal hypothetical alloys from zircon family. <i>Applied Physics A: Materials Science and Processing</i> , <b>2022</b> , 128, 1	2.6	0
2	An extensive computational report on the quinary alloys Cu <sub>2</sub> Zn <sub>1-x</sub> Cd <sub>x</sub> SnS <sub>4</sub> for the solar cell systems: DFT simulation. <i>Computational Condensed Matter</i> , <b>2022</b> , 31, e00670	1.7	0
1	Electronic structure of short-period ZnSe/ZnTe superlattices based on DFT calculations. <i>Condensed Matter Physics</i> , <b>2022</b> , 25, 13701	1.3	