# Habib Rached

## List of Publications by Year in Descending Order



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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 | Theoretical Insight into the Stability, Magneto-electronic and Thermoelectric Properties of XCrSb (X: Fe, Ni) Half-Heusler Alloys and Their Superlattices. *Journal of Superconductivity and Novel Magnetism*, **2022**, 35, 875 | 1.5 | 1 |
| 59 | Electronic structure of short-period ZnSe/ZnTe superlattices based on DFT calculations. *Condensed Matter Physics*, **2022**, 25, 13701 | 1.3 | |
| 58 | 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 | 2.6 | 0 |
| 57 | An extensive computational report on the quinary alloys Cu2Zn1−xCdxSnS4 for the solar cell systems: DFT simulation. *Computational Condensed Matter*, **2022**, 31, e00670 | 1.7 | 0 |
| 56 | 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 | 3.7 | 1 |
| 55 | Electronic structure, magnetic and structural properties of binary cubic C15 Laves phases PrX2 (X = Co and Fe): a first-principles study. *Applied Physics A: Materials Science and Processing*, **2021**, 127, 1 | 2.6 | 0 |
| 54 | Computational determination of structural, electronic, magnetic and thermodynamic properties of Co2HfZ (Z = Al, Ga, Si and Sn) full Heusler compounds for spintronic applications. *Journal of Alloys and Compounds*, **2021**, 894, 162503 | 5.7 | 3 |
| 53 | Prediction of a new quaternary Heusler alloy within a good electrical response at high temperature for spintronics applications: DFT calculations. *International Journal of Quantum Chemistry*, **2021**, 121, e26647 | 2.1 | 5 |
| 52 | Electronic, optical, magnetic and thermoelectric properties of CsNiO(_{mathrm {mathbf {2}}}) and CsCuO(_{mathrm {2}}): Insights from DFT-based computer simulation **2021**, 95, 1 | | 1 |
| 51 | Investigation of Structural, Elastic, Electronic, Magnetic and Thermoelectric Proprieties for Mn2RhZ (Z = Al, Si and Ge) Full-Heusler Alloys. *International Journal of Thermophysics*, **2021**, 42, 1 | 2.1 | 3 |
| 50 | The half metallic behavior at high temperature of highly spin-polarized V-based Heusler alloy: DFT calculations. *European Physical Journal B*, **2021**, 94, 1 | 1.2 | 1 |
| 49 | Ab-initio prediction of high TC half-metallic ferrimagnetism in Li-based Heusler compounds Mn2LiZ (Z= Si, Ge and Sn). *Computational Condensed Matter*, **2021**, 27, e00557 | 1.7 | 7 |
| 48 | Electronic structure and optoelectronic behavior of MgPbP2 chalcopyrite. *Computational Condensed Matter*, **2021**, 27, e00550 | 1.7 | 1 |
| 47 | Prediction of a new Sn-based MAX phases for nuclear industry applications: DFT calculations. *Materials Today Communications*, **2021**, 27, 102233 | 2.5 | 3 |
| 46 | First-principles calculations to investigate structural stabilities, mechanical and optoelectronic properties of NbCoSn and NbFeSb half-Heusler compounds. *International Journal of Quantum Chemistry*, **2021**, 121, e26582 | 2.1 | 10 |
| 45 | 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, 2150007 | 1.3 | 4 |
| 44 | The Vanadium-doping effect on physical properties of the Zr2AlC MAX phase compound. *Materials Chemistry and Physics*, **2021**, 260, 124189 | 4.4 | 6 |

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| 43 | 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 | 4.4 | 7 |
| 42 | Prediction of double transition metal (Cr1−xZrx)2AlC MAX phases as thermal barrier coatings: Insight from density functional theory. *International Journal of Quantum Chemistry*, **2021**, 121, e26770 | 2.1 | 3 |
| 41 | Theoretical insight of stabilities and optoelectronic features of Ru-based Heusler alloys: Ab-initio calculations. *Computational Condensed Matter*, **2021**, 28, e00573 | 1.7 | 1 |
| 40 | Spin gapless semiconductor and nearly spin semimetal antiferromagnets: The case of the inverse Heusler compounds Mn2LiZ (Z = Al and Ga). *Materials Research Bulletin*, **2021**, 143, 111461 | 5.1 | 2 |
| 39 | Investigation of Ruthenium based Full-Heusler compound for thermic, spintronics and thermoelectric applications: DFT computation. *Materials Science in Semiconductor Processing*, **2021**, 134, 106047 | 4.3 | 5 |
| 38 | 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 | 1.7 | 0 |
| 37 | Pressure effects on the structural, elastic, magnetic and thermodynamic properties of Mn2AlC and Mn2SiC MAX phases. *Journal of Alloys and Compounds*, **2021**, 885, 160998 | 5.7 | 11 |
| 36 | The Structural, Electronic, Optical and Thermo-Electric Properties of Oxynitride Perovskite CaTaO2N. *Spin*, **2020**, 10, 2050007 | 1.3 | 6 |
| 35 | Insight into the structural, electronic, mechanical and optical properties of inorganic lead bromide perovskite APbBr3 (A= Li, Na, K, Rb, and Cs). *Computational Condensed Matter*, **2020**, 24, e00478 | 1.7 | 4 |
| 34 | Theoretical Studies of the Structural, Electronic and Magnetic Properties of the CoFeCeZ (Z = P, As and Sb) Quaternary Heusler Alloys. *Spin*, **2020**, 10, 2050002 | 1.3 | 9 |
| 33 | 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 | 1.2 | 14 |
| 32 | Spin Gapless Semiconductor Behavior in d?-d Half-Heusler CrSbSr: Potential Candidate for Spintronic Application. *Spin*, **2020**, 10, 2050025 | 1.3 | 10 |
| 31 | 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 | 1.7 | 12 |
| 30 | Study of the structural, mechanical and thermodynamic properties of the new MAX phase compounds (Zr1-xTix)3AlC2. *Computational Condensed Matter*, **2020**, 23, e00468 | 1.7 | 18 |
| 29 | Full potential study of the structural, electronic and optical properties of (InAs)m/(GaSb)n superlattices. *Computational Condensed Matter*, **2019**, 21, e00394 | 1.7 | 5 |
| 28 | DFT calculations of structural, optoelectronic and thermodynamic properties of BxAl1-xP alloys. *Computational Condensed Matter*, **2019**, 19, e00377 | 1.7 | 5 |
| 27 | 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 | 1.7 | 1 |
| 26 | Magneto-electronic, mechanical and thermodynamic properties of full-Heusler alloys Cr2GdGe1-xSnx. *Journal of Alloys and Compounds*, **2018**, 742, 736-750 | 5.7 | 12 |

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| 25 | First-Principle Study of Half-Metallic Ferrimagnet Behavior in Titanium-Based Heusler Alloys Ti2FeZ (Z = Al, Ga, and In). *Journal of Superconductivity and Novel Magnetism*, **2018**, 31, 1059-1065 | 1.5 | 11 |
| 24 | 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 | 4.4 | 37 |
| 23 | Ab Initio Study of Electronic Structure, Elastic and Transport Properties of Fluoroperovskite LiBeF3. *Journal of Electronic Materials*, **2017**, 46, 2205-2210 | 1.9 | 13 |
| 22 | A Comparative Study of Structural Stability and Mechanical and Optical Properties of Fluorapatite (Ca5(PO4)3F) and Lithium Disilicate (Li2Si2O5) Components Forming Dental Glass□Ceramics: First Principles Study. *Journal of Electronic Materials*, **2016**, 45, 5082-5095 | 1.9 | 23 |
| 21 | Elastic and electronic properties calculations of the filled skutterudite CeOs4P12. *Journal of Physics: Conference Series*, **2016**, 758, 012010 | 0.3 | 2 |
| 20 | Investigation of electronic structure, magnetic properties and thermal properties of the new half-metallic ferromagnetic full-Heusler alloys Cr2GdSi1□Gex: An ab-initio study. *Journal of Alloys and Compounds*, **2016**, 676, 440-451 | 5.7 | 22 |
| 19 | 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 | 1.1 | 5 |
| 18 | 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 | 0.6 | 18 |
| 17 | Electronic structure and optical properties of (BeTe)n/(ZnSe)m superlattices. *Materials Science-Poland*, **2016**, 34, 115-125 | 0.6 | 7 |
| 16 | Theoretical investigation of the structural, electronic, magnetic and elastic properties of binary cubic C15-Laves phases TbX2 (X = Co and Fe). *Journal of Alloys and Compounds*, **2016**, 689, 885-893 | 5.7 | 23 |
| 15 | Electronic structure and magnetic properties of quaternary Heusler alloys CoRhMnZ (Z□=□Al, Ga, Ge and Si) via first-principle calculations. *Journal of Alloys and Compounds*, **2015**, 647, 276-286 | 5.7 | 73 |
| 14 | 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 | 2.8 | 83 |
| 13 | A first principle study of phase stability, electronic structure and magnetic properties for Co2□CrxMnAl Heusler alloys. *Journal of Magnetism and Magnetic Materials*, **2015**, 379, 84-89 | 2.8 | 22 |
| 12 | Computational study of structural, elastic and electronic properties of lithium disilicate (Li(2)Si(2)O(5)) glass-ceramic. *Journal of the Mechanical Behavior of Biomedical Materials*, **2014**, 32, 345-350 | 4.1 | 33 |
| 11 | 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 | 4.4 | 20 |
| 10 | First-principles calculations of the elastic, and electronic properties of YFe2, NiFe2 and YNiFe4 intermetallic compounds. *Computational Materials Science*, **2013**, 73, 56-64 | 3.2 | 8 |
| 9 | Structural, electronic and mechanical properties of RuO2 from first-principles calculations. *Materials Science in Semiconductor Processing*, **2012**, 15, 331-339 | 4.3 | 16 |
| 8 | 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 | 3.2 | 9 |

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| 7 | Structural stabilities, elastic, and electronic properties of iridium mononitride: a first-principles study. *Phase Transitions*, **2011**, 84, 269-283 | 1.3 | 5 |
| 6 | Prediction of stabilities phase and elastic properties of Palladium Carbide. *Computational Materials Science*, **2010**, 48, 556-562 | 3.2 | 14 |
| 5 | 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 | 3.9 | 13 |
| 4 | 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 | 2.8 | 43 |
| 3 | First-principles calculations of structural, elastic and electronic properties of Ni2MnZ (Z = Al, Ga and In) Heusler alloys. *Physica Status Solidi (B): Basic Research*, **2009**, 246, 1580-1586 | 1.3 | 59 |
| 2 | Prediction study of the structural, elastic, electronic and optical properties of the antiperovskite BiNBa3. *Solid State Communications*, **2009**, 149, 2002-2006 | 1.6 | 15 |
| 1 | Elastic stability, electronic structure and optical properties of PtN2 with pyrite and fluorite structures. *Journal of Alloys and Compounds*, **2009**, 478, 297-302 | 5.7 | 6 |