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MALAYSIA.

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Academic Qualification:

Ph.D. (Computational Physics) (2014) – Universiti Teknologi MARA, MALAYSIA.

B. Sc (Hons) Physics (2006-2009) - Universiti Teknologi MARA, MALAYSIA

Working Experiences:

2014 - Present : **Senior Lecturer**
Faculty of Applied Sciences, Universiti Teknologi MARA (UiTM)

**Trainer Consultant for CASTEP Computer Code- Material Studio
: Software**

Workshop Trainer at Universiti Sains Malaysia (USM), Universiti Teknologi Malaysia (UTM), Universiti Kebangsaan Malaysia (UKM) Universiti Teknologi Petronas (UTP), Universiti Teknikal Malaysia Melaka (UTeM) and Universiti Tenaga Nasional (UNITEN)

Service to the University and Professional Memberships:

- **Theoretical and Computational Postgraduate Physics Lab**, Faculty of Applied Sciences, UiTM (Since 2014)
- **Member**, Electroactive Materials Society (EMS): Since 2012
- **Life Member** of Malaysian Solid State Science and Technology Society (MASS): Since 2015

Research Interests:

Computational Materials Science (First Principles and Ab-Initio using DFT) of Ferroelectric, Multiferroic, Batteries (Lithium cathode material), Nano Material (CNT, Graphene) , Heusler Alloy, Sensors, Solar Cell, Superconductor

Invention Awards:

1. **IIDEX 2018- Gold Medal** G-BIOPOLY Storage
2. **IIDEX 2018- Silver Medal** Studies Of Flexible And High Energy Output Nanogenerator Based On $\text{BATiO}_3/\text{GO}/\text{Cellulose}$ Nanocomposites
3. **IIDEX 2018- Silver Medal** The Application of Graphene in DNA-based and Enzyme-based Biosensors
4. **IIDEX 2018- Bronze Medal** Designing Sustainable TiO_2 Solar Cells Materials
5. **ITEX 2017- Gold Medal: 11-13 Mei 2017-)**: A Green Route of Graphene for Energy Harvesting/Storage Devices and Printed Electronics
6. **IIDEX 2017- Gold Medal: 25-29 September 2017-** Nanocomposite Polymer Gel Electrolyte For Lithium Battery
7. **IIDEX 2017- Silver Medal: 25-29 September 2017-** Computational Design of a New Room Temperature Multiferroic Material: Role of ionic Radius in $\text{Bi}_{1-x}\text{Ga}_x\text{FeO}_3$ Solid Solutions
8. **IIDEX 2016- Grand Award (RM 2,000): 20-23 September 2016 -Invention, Innovation and Design Exposition 2016 (IIDEX):** A Green Route of Graphene for Energy Harvesting/Storage Devices and Printed Electronics
9. **IIDEX 2016- Diamond Award Innovation (Inventor) (RM 1,000): 20-23 September 2016-** A Green Route of Graphene for Energy Harvesting/Storage Devices and Printed Electronics
10. **IIDEX 2016- Gold Medal: 20-23 September 2016-** A Green Route of Graphene for Energy Harvesting/Storage Devices and Printed Electronics
11. **IIDEX 2016- Gold Medal: 20-23 September 2016-** The Application of Graphene in Enzyme-based and DNA-based Biosensors

12. **IIDEX 2016- Gold Medal:** 20-23 September 2016- Energy Conversion from Biodegradation of Algae Biomass
13. **IIDEX 2016- Gold Medal:** 20-23 September 2016- Computational Design and Discovery of Novel Multiferroic BiVO_3 : A Quantum Mechanical Ab-initio Approach
14. **NIIDR2015 – Silver Medal:** 23 November 2015 – Energy Conversion From Biodegradation of Algae Biomass
15. **ITEX2014 – Gold Medal:** 10 May 2014 – Green Composite Cellulose Acetate Polymer Electrolytes (G-CAPE) for Lithium Batteries
16. **MTE 2014 – Silver Medal:** 22 Feb 2014 - Green Composite Cellulose Acetate Polymer Electrolytes (CAPE) for Application in Electrochemical Devices
17. **MTE 2014 – Bronze Medal:** 22 Feb 2014 - MG30 Bio-Polymer Electrolytes for Lithium Batteries
18. **PECIPTA 2013 – Bronze Medal:** 09 Nov 2013 – Dispersed Semiconductor Polymer Electrolytes for Solar Cells
19. **MTE 2011 - Silver Medal:** 18 Feb 2011 – Cellulose-Based Solid Polymer Electrolytes for proton Batteries
20. **MTE 2011 - Bronze Medal:** 18 Feb 2111 – Cellulose-Based Solid Polymer Electrolytes for Electrochemical Devices
21. **IID-2010 SE -Innovation and Design Exhibition Bronze Medal:** 14 Oct 2010 – Green Batteries from Cellulose

PhD. Students:

1. **Mohd Fadhlul Wafi Bin Badrudin** – *First Principle Study of Polyanionic LiFeSO_4 and LiFeSO_4OH Cathode Materials Using Density Functional Theory (Ph.D.-completed 2016)*
2. **Mohd Sazwan Affendi Bin Rasiman** – *The Investigation of Cathode Materials of $\text{Li}_2\text{MP}_2\text{O}_7$ ($M=\text{Mn, Fe, Co}$) Family for Battery Application Via First Principles Study (Ph.D.-expected completion 2019)*
3. **Dzulkhairi Taiuddin Bin Mustafa** -- *Theoretical Studies On The Relationship Of Crystal Structure And Band Gaps Of ZnO Nanorods Of Different Aspect Ratios (Ph.D.-expected completion 2018)*
4. **Nur Hafiz Bin Hussin** -- *First Principles Study Toward Lead Free Sn^{2+} And La^{3+} Doped PZT Using Density Functional Theory (Ph.D.-expected completion 2018)*
5. **Mohd Hazrie Bin Samat** – *Theoretical And Experimental Studies On TiO_2 Dispersed With Gd_2O_3 : Er, Nd For Dye Sensitized Solar Cells (Ph.D.-expected completion 2018)*
6. **Nur Hamizah Binti Zaki** – *Preparation and Characterization of Graphene Nanocomposite Electrode Material for Supercapacitors (Ph.D.-expected completion 2019)*
7. **Muhammad Noor Syazwan Bin Saimin** – *First Principles Study On Structural, Electronic, Elastic And Magnetic Properties Of Co_2FeSi Heusler Alloy (Ph.D.-expected completion 2019)*
8. **Maziidah Binti Hamidi** -- *Studies On $\text{Li}_2(\text{Fe}_{1-y}\text{Mn}_y)\text{P}_2\text{O}_7$ ($Y=0,0.5,1.0$) Cathode Materials For Lithium Ion Batteries (Ph.D.-expected completion 2019)*
9. **Maisaratul Shamimi Binti Muhamad Shukri** – *First Principles Study Of Structural, Electronic And Magnetic Properties Of Graphene (Ph.D.-expected completion 2019)*
10. **Lili Widarti Zainuddin-** *First Principles Study on structural and Electronic of LiNbO_3 (Ph.D.-expected completion 2021)*

MSc.Students:

1. **Radhiah Binti Mohd Nor** -- *Investigation On The Effect Of Incorporating ZrO_2 And TiO_2 On The Electrical And Optical Properties Of Terbium-Doped SiO_2 Glass Via Experimental And First Principles Study (MSc.-completed 2018)*
2. **Siti Nabilah Binti Mohd Halim** – *Investigation On The Effect Of Incorporating ZrO_2 And Al_2O_3 On The Electrical And Optical Properties Of Terbium-Doped SiO_2 Glass Via Experimental And First Principles Study (MSc.-completed 2018)*
3. **Nursyazwani Binti Suhaili** -- *First Principles Study Of Organometal Halide Perovskites For Photovoltaic Applications (MSc.-expected completion 2019)*
4. **Nurul Syahirah Binti Azhar** – *First Principles Study Of Ternary Transition Metal For Counter Electrode In Dye Sensitized Solar Cells (MSc.-expected completion 2019)*
5. **Roslan Bin Husin** -- *Electronic, Structure And Optical Properties Of Lithium Niobate Based Sensor For Military Application: A First Principle Study (MSc.-expected completion 2019)*
6. **Kamaliati Hanum Binti Kamaruddin** – *Electronic Energy Band Structure of Electron doped $b\text{Fe}_x\text{Ni}_{1-x}$ ($b=\text{Li, K or Ba}$) Superconductor (MSc.-expected completion 2017)*
7. **Roszaierawani Binti Mohd Ghazali** – *Studies the Properties of Tin Dioxide (SnO_2) using First Principles Calculation Method (MSc.-expected completion 2019)*
8. **Muhammad Zamir Bin Mohyedin** – *First Principles Study of Thermoelectric Performance Between Bi_2Se_3 , Bi_2Te_3 and Sb_2Te_3 By Using Density Functional Theory (MSc.-expected completion 2019)*
9. **Fatin Nabilah Binti Sazman** – *First Principles Study on Prussian Blue for Potassium Ion Battery (MSc.-expected completion 2019)*
10. **Noor Atiqah Binti Md Nasir** – *First Principles Study on Prussian Blue for Sodium Ion Battery (MSc.-expected completion 2019)*

11. **Muhammad Syahir Bin Sak Ari-** *Biopolymer Electrolyte Based on Chitosan : Agarose and 1-Ethyl-3-Methylimidazolium Acetate Ionic Liquid Impregnated with Lithium Bis(Oxalato)Borate* (**MSc.**-expected completion 2020)
12. **Aqeel Bin Idrus –** *First Principle Study on Novel Cathode Material NaFeSO₄OH by using Density Functional Theory* (**MSc.**-expected completion 2020)

RESEARCH GRANTS:

(IN PROGRESS)

1. Thermoelectric Properties Characteristic of X_2Y_3 ($X=\text{Sb, Bi}$; $Y=\text{Te, Se}$) Topological Insulator – **Leader of Project** 600-IRMI/FRGS 5/3 (031/2017) **RM 69,112.00** Ogos 2017 – Ogos 2019
2. Defects Mechanism of Cathode $\text{Li}_2\text{Mn}_2\text{O}_7$ Crystal Structure as-substituted by Transition Metals toward Excellent Current Collector – **Member** of Project FRGS/1/2015/TK05/UITM/02/1) **RM 109,000.00** Nov 2015 – Nov 2017
3. Electron Transport Mechanism of Graphene-Zinc Oxide Semiconductor in Electron Injection of Dye-sensitized solar cells – **Member** of Project FRGS/1/2015/SG06/UITM/02/2) **RM 108,200.00** Nov 2015 – Nov 2017
4. Interaction Mechanism of ZnS/CdSe Semiconducting Quantum Dot in Recombination Process of DSSC – **Member** of Project 600-RMI/FRGS 5/3 (111/2015) **RM 116,200.00** Nov 2015 – Nov 2017
5. Electroactive Materials Research Group – Member of Project 600-RMI/DANA 5/3/REI (14/2015) **RM 32,000.00** Jun 2015 – May 2018
6. Nano-Layer Barium Titanate Adaptive High Frequency Dielectric-Permittivity – **Member** of Project 600-RMI/NRGS 5/3 (4/2013) **RM 521,000.00** Dec 2013 – Nov 2018
7. Experimental and Ab-Initio Studies of Effects of Gallium Substitution on Structural Phase Instability, Electronic and Multiferroic Properties in Nanoparticles $\text{B}_{1-x}\text{Ga}_x\text{FeO}_3$ – **Member** of Project 600-IRMI/FRGS 5/3 (75/2016) **RM 78,600.00** Aug 2016 – Jul 2018
8. Lattice Expansion of $\text{Ba}(\text{Ce,Zr})\text{O}_3$ Ceramic Electrolyte at Intermediate Temperatures-D Proton Conductor – **Member** of Project 600-IRMI/TRGS 5/3 (001/2016) **RM 100,000.00** Dec 2016 – Nov 2019
9. Structural and Electronic Properties of Normal Spinel Cobalt Oxide Doped Cadmium Graphene Composite Electrodes – Member of Project 600-IRMI/FRGS 5/3 (043/2017) **RM 63,600.00** Aug 2017 – Aug 2019
10. Study of Spin Polarization Distribution Co_2FeSi and Co_2FeSiX ($X=\text{Ag, Pt}$) Heusler Alloy – Member of Project 600-IRMI/FRGS 5/3 (047/2017) **RM 66,780.00** Aug 2017 – Aug 2019

(COMPLETED)

1. First Principles and Experimental Approach of Heusler Alloys Co_2FeX ($X=\text{Al, Si, Ge}$ and Ga) – **Leader of Project** RAGS/1/2015/SG0/UITM/02/1) **RM 51,000.00** Dec 2015 – Nov 2017
2. Ab Initio and Experimental Studies On Properties of Lead Free Ferroelectric Materials – **Member** of Project 600-RMI/ST/FRGS 5/3/Fst (4/2010) **RM 45,600.000** 1 Apr 2010-31 Mac 2012
3. Preparation And Characterization Of Lithium Based Glass-Ceramics Conductor Materials For Lithium Batteries- **Member** of project FRGS (600 RMI/ST/FRGS 5/3/Fst (23/2009) **RM 40,000.00** Aug 2009 – Aug 2011
4. Characterization of Graphene Nanocomposites Electrode Materials Supercapacitor – **Member** of Project 600-RMI/RAGS 5/3 (23/2014) **RM 80,000.00** Dec 2014 – Nov 2016.
5. First Principles and Experimental Approach of Heusler Alloys Co_2FeX ($X=\text{Al, Si, Ge}$ and Ga) – **Leader of Project** RAGS/1/2015/SG0/UITM/02/1) **RM 51,000.00** Dec 2015 – Nov 2017
6. Defects Mechanism of Cathode $\text{Li}_2\text{Mn}_2\text{O}_7$ Crystal Structure as-substituted by Transition Metals toward Excellent Current Collector – **Member** of Project FRGS/1/2015/TK05/UITM/02/1) **RM 109,000.00** Nov 2015 – Nov 2017
7. Electron Transport Mechanism of Graphene-Zinc Oxide Semiconductor in Electron Injection of Dye-sensitized solar cells – **Member** of Project FRGS/1/2015/SG06/UITM/02/2) **RM 108,200.00** Nov 2015 – Nov 2017
8. Interaction Mechanism of ZnS/CdSe Semiconducting Quantum Dot in Recombination Process of DSSC – **Member** of Project 600-RMI/FRGS 5/3 (111/2015) **RM 116,200.00** Nov 2015 – Nov 2017

YEAR 2018

1. N Kamarulzaman, DT Mustafa, NF Chayed, N Badar, **MFM Taib**, ABMA Ibrahim, *Comparison of experimental and first-principle results of band-gap narrowing of MgO nanostructures and their dependence on crystal structural parameters*, **Applied Nanoscience**, 1-8
2. M.A. Saad, N.S. Samsi, O.H. Hassan, M.Z.A. Yahya, **M.F.M. Taib**, R. Zakaria, *Studies of the absorbance peak on the N719 dye influence by combination between cadmium selenide (CdSe) QDs and zinc sulphide (ZnS) QDs*, **MATEC Web of Conferences**, Vol. 154 (2018) 01040
3. M.A. Saad, N.S. Samsi, O.H. Hassan, M.Z.A. Yahya, **M.F.M. Taib**, R. Zakaria, *Quantum dot solar cell studies on the influence of cadmium selenide (CdSe) QDs and the zinc sulphide (ZnS) QDs in photoanode*, **MATEC Web of Conferences**, Vol. 154 (2018) 01039

YEAR 2017

4. M.K. Rahman, S.N.M. Halim, R.M. Nor, N. Iznier Razaki, **M.F.M. Taib**, Abdel-baset M. A. Ibrahim, P. Poopalan, *Effects of intrinsic defects on the electronic and optical properties of amorphous silica: first principle study*, **2nd International Conference on Automation, Cognitive Science, Optics, Micro Electro-Mechanical System, and Information Technology (ICACOMIT)**, Vol. 154 (2017) 128-132
5. D.T. Mustafa, N. Kamarulzaman, **M.F.M. Taib**, R. Rusdi, A.B. Ibrahim, *Theoretical investigations of Li⁺ and Co³⁺ positions for layered LiCoO₂ Lithium ion battery cathode material using first principle method*, **AIP Conference Proceedings**, Vol. 1877 (2017) 080005
6. R. Zakaria, A.H. Ahmad, **M.F.M. Taib**, O.H. Hassan, M.Z.A. Yahya, A.M.M Ali, *Correlation studies between surface tension energy and ionic mobility in silicone - Dammar thin film for dye sensitized solar cells*, **AIP Conference Proceedings**, Vol. 1877 (2017) 050002
7. M.A. Azam, F.M. Alias, L.W. Tack, R.N.A.R. Seman, **M.F.M. Taib**, *Electronic properties and gas adsorption behaviour of pristine, silicon-, and boron-doped (8, 0) single-walled carbon nanotube: A first principles study*, **Journal of Molecular Graphics and Modelling**, Vol. 75 (2017) 85-93
8. K. Harun, M.K. Yaakob, **M.F.M. Taib**, B. Sahraoui, Z.A. Ahmad, A.A. Mohamad, *Efficient diagnostics of the electronic and optical properties of defective ZnO nanoparticles synthesized using the sol-gel method: Experimental and theoretical studies*, **Materials Research Express**, Vol. 4 (8) (2017) 085908
9. N.H. Hussin, **M.F.M. Taib**, O.H. Hassan, M.Z.A. Yahya, *Theoretical study of PbZrTiO₃ and PbSnZrTiO₃ using a total-energy planewave-pseudopotential method*, **Materials Research Express**, Vol. 4 (7) (2017) 074001
10. A.A. Mohamad, M.S. Hassan, M.K. Yaakob, **M.F.M. Taib**, F.W. Badrudin, O.H. Hassan, M.Z.A. Yahya, *First-principles calculation on electronic properties of zinc oxide by zinc-air system*, **Journal of King Saud University - Engineering Sciences**, Vol. 29 (3) (2017) 278-283
11. D.T. Mustafa, N. Kamarulzaman, N.F. Chayed, N.H. Badar, **M.F.M. Taib**, A.B.M. Ibrahim, *Particle size dependency of cubic MgO towards its electronic structures, a first principle study*, **Journal of Computational and Theoretical Nanoscience**, Vol. 14 (6) (2017) 2591-2595
12. M.H. Samat, **M.F.M. Taib**, O.H. Hassan, M.Z.A. Yahya, A.M.M. Ali, *Structural, electronic and optical properties of brookite phase titanium dioxide*, **Materials Research Express**, Vol. 4 (4) (2017) 044003
13. M.H. Ridzwan, M.K. Yaakob, **M.F.M. Taib**, A.M.M. Ali, O.H. Hassan, M.Z.A. Yahya, *Investigation of structural, electronic and optical properties of hexagonal LuFeO₃ using first principles LDA + U*, **Materials Research Express**, Vol. 4 (4) (2017) 044001
14. N.S. Azhar, **M.F.M. Taib**, O.H. Hassan, M.Z.A. Yahya, A.M.M. Ali, *Structural, electronic and optical properties of Bi₂O₃ polymorphs by first-principles calculations for photocatalytic water splitting*, **Materials Research Express**, Vol. 4 (3) (2017) 034002

15. R.M. Nor, S.N.M. Halim, **M.F.M. Taib**, M.K. Abd-Rahman, *First principles investigation on the structural, electronic and optical properties of amorphous silica glass*, **Solid State Phenomena**, Vol. 268 (2017) 92-96
16. N. Suhaili, **M.F.M. Taib**, M.K. Yaakob, O.H. Hassan, M.Z.A. Yahya, *Properties of Lead-Free Hybrid Organic-Inorganic Halide Perovskite $\text{CH}_3\text{NH}_3\text{BX}_3$ Using Density Functional Theory*, **Materials Today: Proceedings**, Vol. 4 (4) (2017) 5154-5160
17. F.W. Badrudin, **M.F.M. Taib**, R.I.P.R. Mustapha, O.H. Hassan, M.Z.A. Yahya, *Effects of Vanadium Substitution in the Layered LiFeSO_4OH : A First Principles Investigation*, **Materials Today: Proceedings**, Vol. 4 (4) (2017) Pages 5108-5115
18. R.M. Nor, S.N.M. Halim, **M.F.M. Taib**, A.-B.M.A. Ibrahim, M.K. Abd-Rahman, *First principles study on phonon energy in SiO_2 glass with the incorporation of Al_2O_3* , **Solid State Phenomena**, Vol. 268 (2017) 160-164
19. S.N.M. Halim, R.M. Nor, **M.F.M. Taib**, N.I. Razaki, M.H. Mohd Yusoff, M.K. Abd Rahman, *Intrinsic restructuring of defects in amorphous SiO_2 in manipulating electron-trapping levels via first principles study*, **Solid State Phenomena**, Vol. 268 (2017) 155-159
20. N.H. Hussin, **M.F.M. Taib**, M.H. Samat, N. Jon, O.H. Hassan, M.Z.A. Yahya, *Study of structural, electronic and optical properties of lanthanum doped perovskite PZT using density functional theory*, **Applied Mechanics and Materials**, Vol 864 (2017) 127-132

YEAR 2016

21. F. W. Badrudin, **M. F. M. Taib**, O. H. Hassan, M. Z. A. Yahya, *Effect of lithium intercalation on the structural and electronic properties of layered LiFeSO_4OH and layered FeSO_4OH using first-principle calculations*, **Computational Materials Science**, Vol. 119 (2016) 144-151.
22. M. H. Samat, A. M. M. Ali, **M. F. M. Taib**, O. H. Hassan, M. Z. A. Yahya, *Hubbard U calculations on optical properties of 3d transition metal oxide TiO_2* , **Results in Physics**, 2016
23. M. H. Samat, N. H. Hussin, **M. F. M. Taib**, M. K. Yaakob, N. S. Samsi, S. S. S. A. Aziz et al, *Structural, Electronic and Optical Properties of Nd-Doped Anatase TiO_2 for Dye-Sensitized Solar Cells from Density Functional Theory*, **Materials Science Forum**, Vol. 846 (2016) 726-733.
24. M. H. Samat, N. H. Hussin, **M. F. M. Taib**, M. K. Yaakob, N. S. Samsi, S. S. S. A. Aziz, *First-Principles Study on Structural, Electronic and Optical Properties of TiO_2 for Dye-Sensitized Solar Cells Photoanode*. **Materials Science Forum**, Vol. 846 (2016) 719-725.
25. N. H. Hussin, **M. F. M. Taib**, F. W. Badrudin, N. A. Johari, N. Salleh, M. Z. A. Yahya, *...First Principles Study on Structural and Electronic Properties of PZT and PSnZT Using Density Functional Theory*, **Materials Science Forum**, Vol.846 (2016) 734-739.
26. N. H. Hussin, M. N. S. Saimin, N. Salleh, O. H. Hassan, M. Z. A. Yahya, **M. F. M. Taib**, *Investigation on the Effect of La^{3+} Alteration on Structural Properties of Perovskite PbTiO_3 : Total Energy Calculation*, **Key Engineering Materials**.
27. M. N. S. Saimin, Aziz, S. S. S. A. Aziz, A. M. M. Ali, O. H. Hassan, M. Z. A. Yahya, **M. F. M. Taib**, *Structural and Magnetic Study on the Effect of Substitution of Cobalt by d-Valent Elements of Co_2FeSi Heusler Alloy*, **Key Engineering Materials**.
28. K. H. Kamaruddin, A. F. Z. Abedin, N. A. Zabidi, M. Z. A. Yahya, **M. F. M. Taib**, A. N. Rosli, *First Principles Calculation of ϵ -Phase of Solid Oxygen*, **Acta Physica Polonica A** 129 (4), 468-471.
29. K. Harun, N. Mansor, M. K. Yaakob, **M. F. M. Taib**, Z. A. Ahmad, A. A. Mohamad, *On the verification of sol-gel-derived ZnO nanoparticle properties using first-principles calculation*, **Journal of Sol-Gel Science and Technology** 80 (1), 56-67.
30. K. H. Kamaruddin, N. A. Zabidi, A. N. Rosli, M. Z. A. Yahya, **M. F. M. Taib**, *Electronic structure and phase stability of low-temperature $\text{Ba}(\text{Fe}_{1-x}\text{Ni}_x)\text{2As2}$ superconductor*, **AIP Conference Proceedings** 1787 (1), 050010.

YEAR 2015

31. M. K. Yaakob, **M.F.M. Taib**, L. Lu, O. H. Hassan, M. Z. A. Yahya, *Self-interaction corrected LDA + U investigations of BiFeO₃ properties: plane-wave pseudopotential method*, **Materials Research Express**, Vol. 2 (2015), 11.
32. A. A. Mohamad, M.S. Hassan, M. K. Yaakob, **M.F.M. Taib**, F. W. Badrudin, O. H. Hassan, M. Z. A. Yahya, *First-principles calculation on electronic properties of zinc oxide by zinc–air system*, **Journal of King Saud University**, (2015).
33. M. K. Yaakob, **M. F. M. Taib**, O. H. Hassan, M. Z. A. Yahya, *Low-energy phases, electronic and optical properties of Bi_{1-x}La_xFeO₃ solid solution: Ab-initio LDA+U studies*, **Ceramics International**, Vol. 41(2015)10940–10948.
34. F. W. Badrudin, M. S. A. Rasiman, **M. F. M. Taib**, N. H. Hussin, O. H. Hassan, M. Z. A. Yahya, *First Principles Study on Structural and Electronic Properties of LiFeSO₄F Cathode Material for Lithium Ion Batteries*, **Advanced Materials Research**, Vol. 1107 (2015) 508-513.
35. M. S. A. Rasiman, F. W. Badrudin, M. K. Yaakob, **M. F. M. Taib**, A. M. M. Ali, M. Z. A. Yahya, O. H. Hassan, *An Investigation of Structural and Electronic Properties of Novel Cathode Material Li₂MnP₂O₇ and its Delithiated Li_{2-x}MnP₂O₇ (x=1,2): A First Principle Study*, **Advanced Materials Research**, Vol. 1107 (2015) 485-490.
36. M. H. Samat, N. H. Hussin, **M. F. M. Taib**, M. K. Yaakob, N. S. Samsi, S. S. S. A. Aziz, M. Z. A. Yahya, A. M. M. Ali, *First-Principles Study on Structural, Electronic and Optical Properties of TiO₂ for Dye-Sensitized Solar Cell Photoanode*, **Advanced Materials Research (Accepted)**.
37. M. H. Samat, N. H. Hussin, **M. F. M. Taib**, M. K. Yaakob, N. S. Samsi, S. S. S. A. Aziz, M. Z. A. Yahya, A. M. M. Ali, *Structural, Electronic and Optical Properties of Nd-doped Anatase TiO₂ for Dye-Sensitized Solar Cell from Density Functional Theory*, **Advanced Materials Research (Accepted)**.
38. N.H. Hussin, **M. F. M. Taib**, N.A. Johari, N. Salleh, M. Z. A. Yahya, O. H. Hassan, *First Principles Study on Structural and Electronic Properties of PZT and PSnZT Using Density Functional Theory*, **Advanced Materials Research (Accepted)**.
39. F. W. Badrudin, M. Z. A. Yahya, M. S. A. Rasiman, **M. F. M. Taib**, O. H. Hassan, *First Principles Study of Olivine LiFePO₄ Polyanionic Cathode Materials*, **Journal of Thermal Engineering (Submitted, ICES 2015)**.
40. **M. F. M. Taib**, M. K. Yaakob, N. H. Hussin, M. H. Samat, O. H. Hassan, M. Z. A. Yahya, *Structural Changes, Electronic and Optical Properties of BaTiO₃ and BaFeO₃ from First Principles LDA+U Study*, **Journal of Thermal Engineering (Submitted, ICES 2015)**.
41. N. H. Hussin, M. H. Samat, M. N. Saimin, N. Salleh, O. H. Hassan, M. Z. A. Yahya, **M. F. M. Taib**, *Effect of Rare-Earth Doping on Structural, Electronic and Optical Properties of Perovskite PbTiO₃* (Submitted, ICSSST 2015).
42. N. H. Hussin, M. H. Samat, M. N. Saimin, N. Salleh, O. H. Hassan, M. Z. A. Yahya, **M. F. M. Taib**, *First Principles Study of Lanthanum Doped PZT Using Density Functional Theory* (Submitted, ICSSST 2015).
43. M. H. Samat, N. H. Hussin, N. Adnan, **M. F. M. Taib**, O. H. Hassan, M. Z. A. Yahya, A. M. M. Ali, *Structural, Electronic and Optical Properties Study of Brookite TiO₂* (Submitted, ICSSST 2015).
44. M. H. Samat, N. H. Hussin, N. Adnan, **M. F. M. Taib**, O. H. Hassan, M. Z. A. Yahya, A. M. M. Ali, *First-Principles Study on Elastic and Phase Stability of Rutile, Anatase and Brookite TiO₂* (Submitted, ICSSST 2015).
45. N. S. Azhar, M. H. Samat, N. Hamzah, **M. F. M. Taib**, R. Zakaria, O. H. Hassan, M. Z. A. Yahya, A. M. M. Ali, *Structural, Electronics and Optical Properties Study of Gd-doped TiO₂ for Dye-Sensitized Solar Cells* (Submitted, ICSSST 2015).

46. M. N. S. Saimin, **M. F. M. Taib**, O.H. Hassan, M. Z. A. Yahya, *First Principles Study on Structural, Electronic and Magnetic Properties of Co_2FeSi and CoFeSiX ($X = \text{Ag, Pt}$) Heusler Alloys* (**Submitted, ICSSST 2015**).

YEAR 2014

47. M. K. Yaakob, **M. F. M. Taib**, M. S. M. Deni, M. Z. A. Yahya, *Ab Initio on the Structural and Electronic Properties of Bismuth Ferrite Based on Ferroelectric Hexagonal Phase and Paraelectric Orthorhombic Phase, Integrated Ferroelectrics, Vol.155 (2014) 134-142.*
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REVIEWER FOR JOURNALS:

Selected Journal Reviewer (Summary of Appointment):

1. Journal of Materials and Design (Elsevier, Holland)
2. Journal of Materials Research (Cambridge, England)
3. International Journal of Ionics the Science and Technology of Ionic Motion (Springer)
4. Material Research Express (IOPScience, United Kingdom)
5. Material Research MRS-ID conferences (IOPScience, United kingdom)
6. International Journal of Electroactive Materials (Electroactive Materials Society- Penang, Malaysia)
7. Journal of Oil Palm Research (Selangor, Malaysia)