

## MyRA IMPACT ACTIVITIES

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Grade of Position (VK7/DM54/DM52 etc)	DM51
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### BASIC PROFILE

Appointments	Date/Year of Appointment
Lecturer DM52/DM51	31/07/2015
Year of Birth :	03/02/1987
Ph.D Qualification (Year Obtained)	2015

### POSTGRADUATE SUPERVISION

#### ON-GOING POSTGRADUATE (RESEARCH) SUPERVISION (Includes Co-supervision)

	Students Name	Institutions	Year Enrolled	Year End
1	Muhammad Haziq Bin Ridzwan	UiTM	2016	2018
2	Muhammad Safwan Bin Sazali	UiTM	2016	2018

#### On-Going PhD SUPERVISION (Includes Co-supervision)

	Students Name	Institutions	Year Enrolled	Year End
1	Rozilah Binti Rajmi	UiTM	2014	2018
2	Nurulhuda Binti Ahmad	UiTM	2015	2019

## RESEARCH FUNDINGS

### NATIONAL LEVEL ACTIVE RESEARCH FUNDING (MOSTI/FRGS & Others)

	Research Project	Source	Total Funds	Begin Year	End Year
1	<b>Principal Researcher</b> , Experimental and Ab-initio Studies of Effects of Gallium Substitution on Structural, Phase Instability, Electronic and Multiferroic Properties in Nanoparticles Bi <sub>1-x</sub> GaxFeO <sub>3</sub> 600-RMI/FRGS 5/3 (75/2016)	FRGS	RM78,000	2016	2018
2	<b>Co-Researcher</b> , First Principles and Experimental Approach of Heusler Alloys Co <sub>2</sub> FeX (X=Al,Si,Ge and Ga) RAGS/1/2015/SG0/UITM/02/1)	RAGS	RM51,000	2015	2017
3	<b>Co-Researcher</b> , Nano-Layer Barium Titanate Adaptive High Frequency Dielectric-Permittivity 600-RMI/NRGS 5/3 (4/2013)	NRGS	RM521,000	2013	2018
4	<b>Co-Researcher</b> , Characterization of Graphene Nanocomposites Electrode Materials Supercapacitor 600-RMI/RAGS 5/3 (23/2014)	RAGS	RM80,000	2014	2016

**PUBLICATIONS (Only those indexed in IEEE/ISI/SCOPUS)**

**PUBLICATIONS FOR 2017**

- [1] M. H. Ridzwan, **M. K. Yaakob\***, M. F. M. Taib, O. H. Hassan, M. Z. A. Yahya, A. M. M. Ali, *Investigation of Structural, electronic and optical properties of hexagonal LuFeO<sub>3</sub> using first principles LDA+U*, Materials Research Express, 4, 044001 (2017). **Q3, ISI/SCOPUS**
- [2] R. Rozilah, **M. K. Yaakob\***, Z. Mohamed, A. K. Yahya, Effect of on-site Coulomb interaction (U) on the structural and electronic properties of hal-metallic ferromagnetic orthorhombic Pr<sub>0.75</sub>Na<sub>0.25</sub>MnO<sub>3</sub> Manganite: A LDA+U calculation and experimental study, Materials Research Express, 4, 066103 (2017) **Q3, ISI/SCOPUS**
- [3] 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 CH<sub>3</sub>NH<sub>3</sub>BX<sub>3</sub> Using DFT, **Materials Today: Proceedings**, 4, 5154-5160 (2017) **ISI/SCOPUS**
- [4] K. Harun, N. Mansor, **M. K. Yaakob**, M. F. M. Taib, Z. A. Ahmad, A. A. Mohamad, First Principles Calculation on Electronic Properties of Zinc Oxide by Zinc-air System, Journal of King Saud University – Engineering Sciences 29, 278–283 (2017) **Q1, ISI/SCOPUS**
- [5] K. Harun, N. Mansor, **M. K. Yaakob**, M. F. M. Taib, Z. A. Ahmad, A. A. Mohamad, Efficient Diagnostics on Electronic and Optical Properties of Defective Nanoparticle ZnO Synthesis by Sol-gel Method: Theoretical and Experimental Studies, Materials Research Express, (Accepted) **Q3, ISI/SCOPUS**

**PUBLICATIONS FOR 2016**

- [6] N. S. A. Satar, A. W. Aziz, **M. K. Yaakob (Corresponding Author)**, M. Z. A. Yahya, O. H. Hassan, T. I. T. Kudin, N. H. M. Kaus, Experimental and First-principles Investigations of Lattice Strain Effect on Electronic and Optical Properties of Biotemplated BiFeO<sub>3</sub> Nanoparticles, Journal of Physical Chemistry C, 120, 26012-26020 (2016). **Q1, ISI/SCOPUS**
- [7] 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 TiO<sub>2</sub> for Dye-Sensitized Solar Cell Photoanode*, **Advanced Materials Research (Accepted)** **ISI/SCOPUS**
- [8] 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 TiO<sub>2</sub> for Dye-Sensitized Solar Cell from Density Functional Theory*, **Materials Science Forum 846**, 726-733 (2016) **ISI/SCOPUS**
- [9] 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 CH<sub>3</sub>NH<sub>3</sub>BX<sub>3</sub> Using DFT, **Materials Today: Proceedings (Accepted)** **ISI/SCOPUS**

**PUBLICATIONS FOR 2015**

- [10] M.S.A. Rasiman, M.F.M. Taib, **M.K. Yaakob**, F.W. Badrudin, A.M.M. Ali, O.H. Hassan, M.Z.A. Yahya, An Investigation of Structural and Electronic Properties of 4 Novel Cathode Material Li<sub>2</sub>MnP2O<sub>7</sub> and Its Delithiated Li<sub>2-x</sub>MnP2O<sub>7</sub> (x=1,2) : A First Principle Study, Advanced Materials Research, 1107 (2015) 485-490.
- [11] **M. K. Yaakob**, M. F. M. Taib, L. Lu *et al.*, "Self-interaction corrected LDA + U investigations of BiFeO<sub>3</sub> properties: plane-wave pseudopotential method," *Materials Research Express*, vol. 2, no. 11, pp. 116101, 2015.
- [12] **M. K. Yaakob**, M. F. M. Taib, O. H. Hassan *et al.*, "Low-energy phases, electronic and optical properties of Bi<sub>1-x</sub>LaxFeO<sub>3</sub> solid solution: Ab-initio LDA+U studies," *Ceramics International*, vol. 41, no. 9, Part A, pp. 10940-10948, 2015

**PUBLICATIONS FOR 2014**

- [1] **M. K. Yaakob**, M. F. M. Taib, M. S. M. Deni, and M. Z. A. Yahya, "Ab Initio Studies on the Structural and Electronic Properties of Bismuth Ferrite Based on Ferroelectric Hexagonal Phase and Paraelectric Orthorhombic Phase," Integrated Ferroelectrics, vol. 155, pp. 134-142, 2014/07/24 2014. (Q3 Journal, I.F=0.371)
- [2] F.D. Mansor, **M.K. Yaakob**, M.F.M. Taib, T.I.T. Kudin, O.H. Hassan, M.Z.A. Yahya, Influences of Epitaxial Strain and Volume on BaTiO<sub>3</sub> : Ab Initio Total Energy Calculation, Integrated Ferroelectrics, 155 (2014) 91-99. (Q3 Journal, I.F=0.371)
- [3] M.F.M. Taib, **M.K. Yaakob**, F.W. Badrudin, M.S.A. Rasiman, T.I.T. Kudin, O.H. Hassan, M.Z.A. Yahya, First-Principles Comparative Study of the Electronic and Optical Properties of Tetragonal (P4mm) ATiO<sub>3</sub> (A = Pb,Sn,Ge), Integrated Ferroelectrics, 155 (2014) 23-32. (Q3 Journal, I.F=0.371)
- [4] M.S.A. Rasiman, M.F.M. Taib, **M.K. Yaakob**, F.W. Badrudin, T.I.T. Kudin, O.H. Hassan, M.Z.A. Yahya, Determination of Electronic Structure and Band Gap of Li<sub>2</sub>MnP<sub>2</sub>O<sub>7</sub> via First-Principle Study, Integrated Ferroelectrics, 155 (2014) 71-79. (Q3 Journal, I.F=0.371)
- [5] **M.K. Yaakob**, N.H. Hussin, M.F.M. Taib, T.I.T. Kudin, O.H. Hassan, A.M.M. Ali, M.Z.A. Yahya, First Principles LDA+U Calculations for ZnO Materials, Integrated Ferroelectrics, 155 (2014) 15-22. (Q3 Journal, I.F=0.371)
- [6] M.F.M. Taib, M.K. Yaakob, F.W. Badrudin, T.I.T. Kudin, O.H. Hassan, M.Z.A. Yahya, First Principles Calculation of Tetragonal (P4 mm) Pb-free Ferroelectric Oxide of SnTiO<sub>3</sub>, Ferroelectrics, 459 (2014) 134-142. (Q3 Journal, I.F=0.383)
- [7] I.P.A. Bakar, M.H. Hassan, M.K. Yaakob, M.F.M. Taib, A.M.M. Ali, O.H. Hassan, M.S.M. Deni, M.Z.A. Yahya, Self-interaction Correction in Density Functional Theory of Multiferroic Double Perovskite Bi<sub>2</sub>FeCrO<sub>6</sub> Properties, Int. J. Electroactive Mater. 2 (2014) 40 – 45.

## PUBLICATIONS FOR 2013

- [1] M. K. Yaakob, M. F. M. Taib, M. S. M. Deni, A. Chandra, L. Lu, and M. Z. A. Yahya, "First principle study on structural, elastic and electronic properties of cubic BiFeO<sub>3</sub>," Ceramics International, vol. 39, Supplement 1, pp. S283-S286, 2013. (Q1 Journal, I.F=2.086)
- [2] M.F.M. Taib, M.K. Yaakob, O.H. Hassan, A. Chandra, A.K. Arof, M.Z.A. Yahya, First principles calculation on structural and lattice dynamic of SnTiO<sub>3</sub> and SnZrO<sub>3</sub>, Ceramics International, 39, Supplement 1 (2013) S297-S300. (Q1 Journal, I.F=2.086)
- [3] M.F.M. Taib, M.K. Yaakob, O.H. Hassan, M.Z.A. Yahya, Structural, Electronic, and Lattice Dynamics of PbTiO<sub>3</sub>, SnTiO<sub>3</sub>, and SnZrO<sub>3</sub>: A Comparative First-Principles Study, Integrated Ferroelectrics, 142 (2013) 119–127. (Q3 Journal, I.F=0.371)
- [4] M.F.M. Taib, M.K. Yaakob, F.W. Badrudin, T.I.T. Kudin, O.H. Hassan, M.Z.A. Yahya, First Principles Calculation of Tetragonal (P4 mm) Pb-free Ferroelectric Oxide of SnTiO<sub>3</sub>, Ferroelectrics, 452 (2013) 122–128. (Q3 Journal, I.F=0.383)

## PUBLICATIONS FOR 2012

- [1] M. K. Yaakob, M. F. M. Taib, and M. Z. A. Yahya, First Principle Study of Dynamical Properties of a New Perovskite Material Based on GeTiO<sub>3</sub>, Advanced Materials Research, 501 (2012) 352-356.