



## PROF. MADYA DR. AHMAD NAZRUL BIN ROSLI

PENSYARAH UNIVERSITI DS14

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Address: Fakulti Sains Dan  
Teknologi

### SUPERVISION

PhD - Completed: 1, Ongoing: 2

Master - Completed: 1, Ongoing: 0

### AREAS OF EXPERTISE

Other Theoretical And Computational Physics N.e.c  
Condensed Matter Physics

### BIOGRAPHY

A lecturer from Fakulti Sains Dan Teknologi. Holds a Phd in Fizik.

### ACADEMIC QUALIFICATION

Phd in Fizik (2011)  
Master in Fizik (2008)  
Bachelor in Fizik Industri (2006)

### RESEARCH

1. A FIRST PRINCIPLES STUDY OF GRAPHENE, GRAPHENE-DOPED METAL AND THE INTERACTION WITH GLUCOSE

2026 ON GOING MAIN RESEARCHER

2. DENSITY FUNCTIONAL THEORY STUDY (DFT) STUDY OF INTERACTIONS BETWEEN PHOTOCATALYST-BIOADSORBENTS (O-PYRITE/CHITOSAN)

2019 COMPLETED MAIN RESEARCHER

3. ELECTRONIC PROPERTIES OF ARSENE LAYER CALCULATED USING DENSITY FUNCTIONAL THEORY

2018 COMPLETED MAIN RESEARCHER

4. AB INITIO CALCULATION OF VIBRATIONAL SPECTRA OF ZINC CLUSTER OF THE STANNITE-KESTERITE AND THE RAMAN SPECTRA

2013 COMPLETED MAIN RESEARCHER

5. DENSITY FUNCTIONAL THEORY (DFT) CALCULATION OF SUPERCONDUCTIVITY OF CAC6, BAC6, YBC6, C6CAC6 AND OTHER GRAPHITE COMPOUNDS

2013 COMPLETED MAIN RESEARCHER

# PUBLICATION

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## 1. PRELIMINARY DFT STUDY OF THE ENERGY GAP OF GINGEROL

2025 PROCEEDING

## 2. SOROTAN 2: KEHILANGAN YANG MENGINSAFKAN

2025 CHAPTER IN BOOK

## 3. THE STRUCTURAL STUDIES OF LAWSONE IN HENNA: THE FIRST PRINCIPLE APPROACH

2024 PROCEEDING

## 4. DETERMINATION OF THERMOELECTRIC PROPERTIES OF FLAT LAYER ARSENENE USING BOLTZMANN TRANSPORT EQUATION: A COMPUTATIONAL STUDY

2022 PROCEEDING

## 5. THE STUDY OF A STRUCTURAL AND ELECTRONIC PROPERTIES OF TWO-DIMENSIONAL FLAT LAYER ARSENENE USING PLANEWAVES DENSITY FUNCTIONAL CALCULATION

2020 JOURNAL

## 6. INTRODUCTION TO VIBRATIONS AND WAVES

2019 BOOK

## 7. THE BAND STRUCTURE OF A RARE EARTH ELEMENT OF PROMETHIUM (III) OXIDE (PM<sub>2</sub>O<sub>3</sub>) CALCULATED USING DENSITY FUNCTIONAL THEORY

2018 JOURNAL

## 8. A FIRST PRINCIPLE STUDY OF BAND STRUCTURE OF TETRAGONAL BARIUM TITANATE

2017 JOURNAL

## 9. DENSITY FUNCTIONAL THEORY (DFT) CALCULATION OF BAND STRUCTURE OF KESTERITE

2015 JOURNAL

## 10. THE STUDY OF BAND STRUCTURE OF GRAPHITE INTERCALATION COMPOUND CONTAINING SODIUM CALCULATED USING DENSITY FUNCTIONAL THEORY

2015 JOURNAL

## 11. THE ELECTRONIC STRUCTURE OF PEROVSKITE-TYPE MATERIAL BARIUM TITANATE (BaTiO<sub>3</sub>) CALCULATED USING DENSITY FUNCTIONAL THEORY (DFT)

2015 PROCEEDING

## 12. AB INITIO CALCULATION OF VIBRATIONAL FREQUENCIES OF ZnSe AND THE RAMAN SPECTRA

2014 JOURNAL

## 13. CLUSTERS OF GaAs PREPARED BY QUANTUM MECHANICAL DFT AND THE NANOWIRE RAMAN SPECTRA

2013 JOURNAL

## 14. DFT CALCULATION OF VIBRATIONS IN THE CLUSTERS OF ZINC AND OXYGEN ATOMS, AHMAD NAZRUL ROSLI, HASAN A. KASSIM, AND KESHAV N. SHRIVASTAVA, SAINS MALAYSIANA, 42 (5) 649-654 (2013).

2013 JOURNAL

15. THE RAMAN SPECTRA OF NANOCOMPOSITE CLUSTERS OF ATOMS IN PHOSPHOROUS-SELENIUM GLASSY STATE, AHMAD NAZRUL ROSLI, HASAN A. KASSIM, KESHAV N. SHRIVASTAVA AND V. RADHIKA DEVI, ADVANCED MATERIALS RESEARCH 667, 99-103 (2013).

2013 JOURNAL

16. AB INITIO CALCULATION OF VIBRATIONAL FREQUENCIES OF ZNSE AND THE RAMAN SPECTRA, AHMAD NAZRUL ROSLI, NORIZA AHMAD ZABIDI AND HASAN ABU KASSIM, AIP CONFERENCE PROCEEDINGS 1588, 265 (2014); DOI: 10.1063/1.4866958.

2013 PROCEEDING

17. CLUSTERS OF GAAS PREPARED BY QUANTUM MECHANICAL DFT AND THE NANOWIRE RAMAN SPECTRA

2012 PROCEEDING

18. DENSITY-FUNCTIONAL THEORY OF VIBRATIONS IN NI<sub>1</sub>-XVX CLUSTERS.

2011 JOURNAL

19. DFT CALCULATION OF CLUSTERS OF BA AND O ATOMS AND THE RAMAN SPECTRA OF BARIUM PEROXIDE.

2011 JOURNAL

20. AB INITIO CALCULATION OF VIBRATIONAL FREQUENCIES OF ASO GLASS.

2010 JOURNAL

21. AB INITIO CALCULATIONS OF VIBRATIONAL FREQUENCIES IN A GLASSY STATE OF SELENIUM.

2010 JOURNAL

22. DFT CALCULATIONS OF VIBRATIONAL FREQUENCIES OF CARBON-NITROGEN CLUSTERS: RAMAN SPECTRA OF CARBON-NITRIDES

2010 JOURNAL

23. DFT CALCULATION OF CLUSTERS OF BA AND O ATOMS AND THE RAMAN SPECTRA OF BARIUM PEROXIDE.

2010 PROCEEDING

24. CLUSTERS OF GE AND O ATOMS AND THE RAMAN SPECTRA OF VITREOUS GEO<sub>2</sub>.

2010 PROCEEDING

25. DENSITY FUNCTIONAL THEORY CALCULATION OF ADSORPTION OF NaCl ON CHLOROPHYLL.

2009 JOURNAL

26. DFT CALCULATION OF VIBRATIONAL FREQUENCIES IN CLUSTERS OF FE AND AS ATOMS

2009 PROCEEDING

27. GRAPHENE INFRARED SPECTROSCOPY: DFT VIBRATIONAL FREQUENCIES

2009 PROCEEDING

28. DFT DETERMINATION OF LAW OF FORCE IN FE AND P CLUSTERS OF ATOMS

2009 PROCEEDING

29. AB INITIO CALCULATION OF VIBRATIONAL FREQUENCIES IN ASX<sub>S1</sub>?X GLASS AND THE RAMAN SPECTRA

2008 PROCEEDING

30. VON KLITZING'S CONSTANT AS A SPECIAL CASE OF GENERALIZED CONSTANTS

2008 PROCEEDING

## AWARDS/RECOGNITION

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## 1. SILVER MEDAL

2025

INTERNATIONAL

## 2. ANUGERAH KUALITI FST 2024

2025

UNIVERSITY

## 3. ANUGERAH LIBATSAMA KOMUNITI (PROJEK SCIFEST)

2025

UNIVERSITY

## 4. TRAINER / FACILITATOR

2025

UNIVERSITY

## 5. IOT-ENABLED NEAR INFRARED SENSOR SYSTEM FOR POLYAMIDE ABSORPTION CHARACTERIZATION

2025

Antarabangsa

Silver