ANOUAR AKACHA DELENDA

PhD student[1]

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PhD thesis

PhD : Dislocations in layered carbon nanomaterials **November 2024 - present**
Institut des Matériaux de Nantes Jean Rouxe, Nantes, France.

• In materials engineering, defects such as dislocations (e.g. in screws and edges) are of fundamental importance. The control of these defects has the potential to drive significant advancements in the field of materials science. However, these defects are not yet fully understood, especially in the case of anisotropic materials. My research focuses on understanding the behaviour of these defects and their impact on layered materials such as graphite. To this end, I utilise atomistic modelling employing Gaussian DFT-based code and molecular dynamic simulation using machine learning interatomic potential.

Education

M.Sc : MASTER Physics of Optics and Photonics **September 2023 - June 2024**
University Claude Bernard Lyon 1, France.
• Master's Degree (Master 2).

M.Sc : MASTER of Condensed Matter and Nanophysics **September 2022 - June 2023**
University of Strasbourg, STRASBOURG FRANCE.
• Master's Degree (Master 2)
• **Ecole Doctoral (ED182-Strasbourg): Succeeded**

M.Sc : MASTER in Materials Physics **2019-2021**
Option: Semiconductors and dielectric materials
University of Science and Technology HOUARI Boumediene Bab Ezzouar, Algiers Algeria.
• Master's Degree (Master 2).
• **Rank:** 1^{st}.

B.Sc : BACHELORS In Fundamental Physics **2016-2019**
University of Science and Technology HOUARI Boumediene Bab-Ezzouar, Algiers Algeria.

Academic experience

A. Conferences

• **Carbon2025**: **June 29^{th} $\longrightarrow$ July 4^{th} 2025** (Proceedings)

Location: Saint-Malo, France.

Description: Each year, scientists from academic and industrial backgrounds who specialise in carbon materials come together to discuss all aspects of this fascinating element. These aspects include the various processes involved in synthesising the materials, as well as their applications, characterisation and understanding of their properties.

Contribution: Submitted poster.

Certification: Participation certificate.

- **NanoteC**: August **27**th $\longrightarrow$ **30**th **2024** (Proceedings)

  Institution: Institut des Matériaux de Nantes Jean Rouxe, Nantes, France..

  Description: The NanoteC is a student friendly international meeting focusing on nanocarbon materials: their production, treatment, properties, in all their monocolour (black) glory! This three days meeting has been running annually, almost continuously since 1998, and in 2024 it took place in Nantes at the Institute of Materials, one of its regular haunts where many previous memorable NanoteCs have taken place.
  During this conference I participated with a poster titled: **Development of a reactive Neural Network Potential for borophene on silver and gold**. A fruitful work of the internship conducted at Laboratoire des Multimatériaux et Interfaces; Matériaux à Basse Dimensionnalité (MBD) team, And Institut Lumière Matière (ILM); Physicochimie théorique team, during my last master in the University Claude Bernard Lyon 1, France. Villeurbane, France.

  Certification: NanoteC24 (Participation certificate).

  Achievement: Best poster award.

- **ICREATA'21**: **October 25**th $\longrightarrow$ **27**th **2021**

  Institution: Research Unit for Renewable Energies in Saharan region, Adrar Algeria.

  Description: THE FIRST INTERNATIONAL CONFERENCE ON RENEWABLE ENERGY ADVANCED TECHNOLOGIES AND APPLICATIONS (ICEATA'21). The video-conference aim was to promote an exchange of recent developments among scientists and engineers, in the various areas of renewable energy. Including solar photovoltaic and others related area.

  Achievement: The Submitted Work : Power Losses Diagnosis In Solar Cells Fabricated At CRTSE. Authors: N. Khelifati, A. A. Delenda, G. Fortas, F. Kezzoula, B. Palahouane and B.Mahmoudi.

  Certification: ICREATA'21 Certification.

B. Workshops

- **Pyroman**: **June 28**th $\longrightarrow$ **29**th **2025** (Proceedings)

  Location: Rennes, France

  Description: Most real-world carbon applications still rely on bulk, disordered materials rather than crystalline nanoforms like graphene. Understanding and modeling the complex structure of these materials across scales remains a major scientific challenge. The workshop titled **Bulk Carbon Materials: processing conditions, structure & properties** aim to bring together experts to discuss recent advances in processing, characterization, and modeling of carbon materials.

  Contribution: Submitted poster.

- **Exploring chemical reactions in VASP**: **November 06**th $\longrightarrow$ **08**th **2024**

  Location: Online.

  Description: Three-day workshop focuses on simulating chemical reactions in VASP, covering both harmonic and anharmonic methods. Objectives are mainly exploring transition state search techniques, including NEB, IDM, and MD-based approaches for rare events. Hands-on sessions with expert guidance was provided to guide apply these methods to real reactions, enhancing participants VASP simulation skills.

  Certification: Proof.

C. Internships

- **05/02/2024 ⟶ 26/07/2024**

  Task: **Identification of borophene allotropes from STM images by Machine Learning: from the development of a neural network interatomic potential to building the image classification tool** (Thesis).

  Institution: Laboratoire des Multimatériaux et Interfaces; Matériaux à Basse Dimensionnalité (MBD) team, And Institut Lumière Matière (ILM); Physicochimie théorique team. Villeurabne, France.

  Description:The purpose of this internship is to use the an existing Neural Network Potential (NNP) in order to create a Database of metal supported Borophene structures.Hereafter, scanning tunneling microscope (STM) images will be simulated to train a Neural Network. for the classification of various Borophene allotropes. The work start on Gold (Au) substrate then will be extended to various metals (Cu, Ir ...).

- **21/02/2023 ⟶ 21/06/2023**

  Task: **Characterization Of Ultrashort Laser Pulse Centred at 800 nm** (Thesis).

  Institution: Department of Ultrafast Optics and Nanophotonics (DON) at the Institute of Materials Physics and Chemistry De Strasbourg (IPCMS). Strasbourg, France.

  Description:Characterization of an Ultra-fast laser pulse centred at 800 nm. Using the Frequency Resolved Optical Gating (FROG) and the Time Domain Ptychography techniques. The problem we solved is a reconstruction problem in particular, spectral phase retrieval. And I Implemented the Time Domain Ptychography algorithm in order to Characterize the ultrashort pulses.

- **15/04/2021 ⟶ 30/06/2021**

  Task: Power Loss Analysis On Based Silicon Solar cells (Thesis abstract)

  Institution: Research Center of Semiconductors Technologies for Energetics (CRTSE). Algiers, Algeria.

  Description: Working on conventional multi-crystalline (m-Si) Solar Cells manufactured at the C.R.T.S.E. After categorizing various origin of the Power Losses of I presented a methodology to quantify these quantities; that occurs at different stages (Layers) of the solar cells.

  Certification: Internship Certification.

Area of Interests

- Solid State of Physics & Nano-Materials Devices (2D Materials);
- Atomistic Simulation;
- Photonics;
- Semiconductors & Opto-electronics Devices;
- Artificial Intelligence: Machine Learning.

Skills & Projects

- **Materials characterization techniques**: Solar simulator, Spectral Response, Suns-Voc etc...
- **Ultrafast Laser characterization**: Interferometric Auto-correlation , Frequency Resolved Optical Gating (FROG) and Time Domain Ptychography.
- **Programming** (Python & Bash), projects examples:
  - Ultrafast Ptychography.
  - Electronic Density calculation
  - Model Selection for Atomization Energy Prediction
  - Covid-19 Data Analysis
- **Atomistic Simulation**:

- Vienna Ab initio Simulation Package (VASP)
- **A**b **I**nitio **M**odelling **PRO**gram (AIMPRO).
- Atomic Simulation Environment(ASE):
  Python based package for building manipulating atomic structures and pipeline interface with DFT codes.
- LAMMPS Molecular Dynamics Simulator
- OVITO - Open Visualization Tool

- **Machine Learning interatomic potential (MLIP)** :
  Such as High Dimensional Neural Network Potential (HDNNP) & Atomic Cluster Expansion (ACE).

References

- Dr. Christophere EWELS:
  CNRS Research Director at the Institute of Materials in Nantes, France. Co-Responsable of Physics of materials and nano-structures (PMN).
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- Dr. Colin Bousige:
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- Dr. Pierre Mignon:
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Additional Links

Link to Certificates and Diplomas.

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