Dr. Djohra Bedghiou

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SUMMARY

Highly motivated and meticulous research scientist experienced in working independently and collaboratively within interdisciplinary teams. Proven ability to thrive under pressure while consistently delivering results. Dedicated to solving challenging problems in computational chemistry through diverse skills and interdisciplinary knowledge.

HIGHLIGHTS

- Modeling and Computer Simulation
- Metadynamics
- Proficient in Linux/Windows operating systems
- Proficient in utilizing USPEX, VASP, Materials Studio, and Phonopy
- Development of New Materials with Specific Properties
- Advanced Photocative Materials
- Strong Supporter and User of Existing Literature
- Proficiency in Languages: Arabic, French, English

Work Style:

- Willing to tackle basic tasks and progress to solving complex problems
- Quick learner, adept at acquiring new knowledge and adjusting to new environments
- Balances independent work effectively with strong teamwork skills
- Demonstrates strong organization skills and genuine passion for the work.

EDUCATION

January 2020

Doctor of Philosophy (PhD), KHENCHELA UNIVERSITY (ALGERIA)

Title: Theoretical Studies of Electronic and Optical Properties of Titanium Dioxide (TiO_2)

June 2012

Master's Degree, KHENCHELA UNIVERSITY (ALGERIA)

Title: Experimental Study of Cyclic Oxidation Behavior of FeAl Alloys in Air at High Temperatures

TRAINING

- IEA-Training certificate in Molecular docking| October 2022| University of Constantine 1
- TICE and teaching practices training | February-November 2021| University of Constantine 1
- University certificate in transversal skills (U2ES) | 2016-2017 | University of Namur
- High performance scientific computing (HPC) training | October-November 2017 | University of Louvain
- Training Courses on Intellectual Properties and Development of Research Results| February 2017 | University of Namur
- Certificate of Quality management - ISO and GLP standards| December 2016 | University of Namur

EXPERIENCE

University Lecturer/ Researcher — Since Oct 2020
Khenchela University — Khenchela, Algeria

- Responsible for designing courses (Fields: Ceramics, Polymers, Spectroscopic Methods, Quantum Chemistry) and running research programs

Supervisor of MSc Students — Since Jan 2019
Khenchela University — Khenchela, Algeria

- Etude théorique et expérimentale du dopage des *blends* à base de TiO_2
- Théorie de la Matière condensée : Etude *in silico*
- Interprétation quantique de la migration électron-trou dans les *blends* TiO_2 dopés
- Etude théorique de l'amélioration photocatalytique des *blends* dopés

Visiting Researcher — Nov 2016 to Jun 2018
University of Namur — Namur, Belgium

- Computational materials discovery: prediction of hyper photoactive TiO_2 compounds under high pressure using density functional theory (VASP) and USPEX evolutionary algorithm. Study of their vibrational, structural, thermodynamic, mechanical and electronic properties *via* CASTEP and Phonopy.
- Formulated an ideal model for anatase–brookite mixed-phase by using a set of novel theoretical methods, including evolutionary metadynamics code (Very powerful method for finding the global minimum) *via* USPEX and PTMC (Phenomenological Theory of Martensite Crystallography) *via* PTCLab code.
- Good knowledge of USPEX code (Finding low-energy metastable phases, stable structures of crystals, nanoparticles, surface reconstructions, molecular packings in organic crystals. Searching materials with desired physical (mechanical, electronic) properties knowing only the chemical composition).
- Good knowledge of VASP (Computer program for atomic scale materials modelling, e.g. electronic structure calculations and quantum-mechanical molecular dynamics, from first principles).

Visiting Researcher — May to Jun 2016
University of Namur — Namur, Belgium

- Proposed to construct a first three-phase atomic model for the anatase–brookite TiO_2 heterophase junction and determine its optical and electronic properties using crystal phase transition pathway sampling, interfacial strain analysis and first principles thermodynamics evaluation of holes and electrons.

- Good knowledge of Materials Studio (Software for simulating and modeling organic, inorganic, and organometallic materials, polymers, oligomers, and peptides. Quantum methods to predict electronic, optical, structural, vibrational and mechanical properties. Molecular dynamics simulation. Scan over wide areas of a potential energy surface or reaction pathway, etc.).

Visiting Researcher **February 8-26, 2016**

University of Namur **Namur, Belgium**

- Good knowledge of CASTEP code (DFT, simulation of energetics, vibrational properties, electronic response properties etc. A wide range of spectroscopic features that link directly to experiment).

Laboratory Assistant **Nov 2010 to Apr 2012**

Salhi-Belkacem Maternity **Khenchela, Algeria**

- Verified patient details on forms and samples
- Prepared specimens and conducted routine and specialized tests
- Prepared and stained slides for analysis
- Recorded testing data
- Managed inventory and ordered lab supplies

CONFERENCES

December 2018

4 èmes Journées Internationales de Chimie Organique, JICOA" 18, ANNABA

Title: Prédiction de structures cristallines TiO_2 par l'algorithme évolutionnaire USPEX : étude de l'évolution de gap optique en fonction de la pression| Type: Oral presentation

June 2018

Kick-off ILEE 2018, NAMUR

Title: Three-phase junction for modulating electron-hole migration in anatase-brookite photocatalysts| Type: Poster

May 2018

HPC Meets Materials Conference 2018, NAMUR

Title: Electronic and optical properties of anatase-TiO2-II-brookite three-phase junction photocatalyst| Type: Poster

June 2017

Journées Théorie, Modélisation et Simulation, JTMS17, PARIS

Title: Electronic and optical properties of anatase-TiO_2-II-brookite three-phase junction photocatalyst| Type: Poster

March 2017

The 43 rd Conference on Phase Equilibrium, JEEP 2017, BARCELONA

Title: Understanding the electron-hole migration in anatase -TiO_2 -II-brookite three phase junction photocatalyst| Type: Oral presentation

PUBLICATIONS

- D. Bedghiou, F. Hamza Reguig and A. Boumaza, Novel high/ultrahigh pressure structures of TiO_2 with low band gaps. Computational Materials Science 166 (2019) 303 https://doi.org/10.1016/j.commatsci.2019.05.016

Currently Under Preparation:

- Three-phase Junction for Modulating Electron–Hole Migration in Anatase/Brookite Photocatalysts. D. Bedghiou, F. Hamza Reguig and A. Boumaza
- Effect of Metal Doping on Electronic Structure and Photocatalytic Properties of TiO_2 Blends D. Bedghiou, F. Hamza Reguig and A. Boumaza
- New Three-dimensional Semiconductors with Ideal Band Gap for Solar Harvesting D. Bedghiou, F. Hamza Reguig and A. Boumaza
- First-principles Study of Ti–O Crystalline Phases: Phase Stability, Electronic and Mechanical Properties. D. Bedghiou, F. Hamza Reguig and A. Boumaza

HOBBIES

- Literature
- History and Ancient Civilizations
- Classical Music
- Theatre
- Gastronomy
- Manga

REFERENCES

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Abdelkader Djelloul
Professor at Khenchela University, Algeria
djelloulabdelkader@yahoo.fr

Farouk Hamza Reguig
Professor at the University of Oran 1, Algeria
hamza_rf70@hotmail.com