

Tentative Outline

Special Thematic Issue for the journal

Advanced Nanomaterials and Nanosystems

Guest Editors: Dr. Dibya Prakash Rai & Dr. Kingsley O. Obodo

- **Scope of the Thematic Issue:**

- ✓ Magnetic materials for Spintronics, data storage and data transfer.
- ✓ Advanced Materials for energy harvest and energy production (including H₂-fuel).
- ✓ 2D materials for gas sensors.
- ✓ Anode/Cathode Materials for rechargeable alkali ion battery.
- ✓ Topological Insulators.
- ✓ Nanomaterials for catalysis, sensors and waste-water treatment
- ✓ Nanomaterials for optoelectronics and mechatronics.
- ✓ Advanced Materials for thermoelectricity and Solar-cell applications.
- ✓ Bio-based nanomaterials for food technology, agriculture, cosmetics, medicine, health, etc.
- ✓ Not limited to only above mentioned topics.

Keywords: *Nanomaterials, Solarcell, Hydrogen evolution reaction (HER), Nano-catalysts, Nano-sensors, Spintronics, Li-ion battery, Topological insulator, Optoelectronics, Thermoelectric, Bio-sensors, Biomaterials.*

Sub-topics:

The sub-topics to be covered within the issue should be provided:

- Chemical Sciences
- Materials Sciences
- Biological Sciences
- Physical Sciences
- Nanotechnology and Nanosciences

Tentative titles of the articles and list of contributors:

Tentative titles of the articles and a list of contributors with their names, designations, addresses and email addresses should be provided.

1. *“Carbon doped hexagonal boron nitride nanosheet for hydrogen storage : A DFT study”*

Dr. D. P. Rai, Assistant Professor, Pachhunga University College, Aizawl, (India)

Email:dibya@pucollege.edu.in

2. *“Environmental health and nanoparticles”*

Dr. R. Tamang, Assistant Professor, Calcutta University, Kolkata (India). Email: rtzoo@caluniv.ac.in

3. *“Density functional theory evaluation of surface segregation in Pt₃Nb and Pt₃Ti.”*

Dr. K. O. Obodo, Assistant Professor, North-West University (NWU), P. Bag X6001, Potchefstroom, 2520, South Africa. Email: obodokingsley@gmail.com

4. *“Opto-electronic and electron transport properties of Boron and Nitrogen doped SWCNT: A first principal study”*

Prof. R. K. Thapa, Retired Professor, Mizoram University, Aizawl (India)

Email:r.k.thapa@gmail.com

5. *"Recent advancement in nanomaterials in n dimensions"*
Prof. M. L. Verma, Professor, Shri Shankaracharya Technical Campus, Bhilai, Chhattisgarh, India. Email: drmohanlv@gmail.com
6. *"C-DFT and Its Applications in the Chemistry"*
Dr. S. Kaya, Associate Professor, Cumhuriyet University, Turkey. Email: Savaskaya1989@gmail.com
7. *"A novel, mesoporous CuO @barley straw-derived SiO₂ nanocomposite for adsorption and photocatalytic degradation of methylene blue from textile wastewater"*
Dr. Mohammed Ezzeldien, Associate Professor, Faculty of Science, South Valley University, Qena, Egypt. Email: meabas@ju.edu.sa
8. *"Mechanism of growth of Sulvanite nanoparticles in solution"*
Prof. I. Oksana, professor, Uzbekistan-Japan Innovation Center of Youth, Tashkent, Uzbekistan. Email: oismailova56@gmail.com
9. *"Electronic and thermoelectric properties of 2D Janus structures"*
Dr. Nguyen N. Hieu, Associate Professor, Institute of Research and Development, Duy Tan University (Vietnam). Email: hieunn@duytan.edu.vn
10. *"Wide bandgap semiconductors properties"*
Dr. U. Bhandari , Research Scholar, Louisiana State University (USA).
Email: bhandari91uttam@gmail.com
11. *"Multiscale study on the structural and thermomechanical properties of ceramic matrix nanocomposites"*
Dr. A. M. Ukpong, Associate Professor, University of KwaZulu-Natal, Pietermaritzburg, South Africa. Email: ukponga@ukzn.ac.za
12. *"Nanostructured carbons for batteries : A review"*
Dr. B. Thangaraj, Postdoctorate Research Associate, King Mongkut's University of Technology Thonburi, Bangkhuntien-chaitalay Road, Thakam, Bangkok-10150, Thailand. Email: thabaskar@gmail.com
13. *"Thermoelectric properties of low dimensional monochalcogenides : First principle calculations"*
Prof. B. Hamad, Professor, The University of Jordan, Amman, 11942, Jordan.
Email: b.hamad@ju.edu.jo
14. *"Electronic and optical properties of co-doped MoS₂ monolayers"*
Dr. Joshua T Obodo, Assistant Professor, University of Nigeria, Nsukka, Nigeria.
Email: einsteindgreat@gmail.com
15. *"Machine learning screening model for gas sensing applications: Insights from transition metal adatoms on Sn₃C₂ monolayer mxene"*
Dr. Cecil N M Ouma, Assistant Professor, North-West University (NWU), P. Bag X6001, Potchefstroom, 2520, South Africa. Email: moronaphtaly84@gmail.com
16. *"Ab initio predictions of half-metallicity, magnetism, dynamical and mechanical properties of Iridium-based Heusler alloys"*
Dr. R. Paudel, Scientist, Nepal Academy of Science and Technology (NAST), Kathmandu, Nepal. Email: r.paudel@qq.com

17. "Magnetic nanoclusters in Cu-III-VI₂/TM-VI alloys (III: Ga, In; VI: Se, Te; TM: Transition Metals)"

Prof. Pedro Grima Gallardo, Professor, Centro de Investigaciones de Astronomia (CIDA), Venezuela.
Email: peg1952@gmail.com

18. "Study of the physical properties of some Heusler quaternary alloys"

Prof. Hakim Baaziz, Professor, Department of Physics, Faculty of Science, University of M'sila, M'sila, Algeria. Email: baaziz_hakim@yahoo.fr

19. "Theoretical study of an AlGaP₂ semiconductor material In photovoltaic applications"

Prof. Hakim Baaziz, Professor, Department of Physics, Faculty of Science, University of M'sila, M'sila, Algeria. Email: baaziz_hakim@yahoo.fr

20. "Study of the electronic structure of semiconductors II-IV -V₂"

Prof. Hakim Baaziz, Professor, Department of Physics, Faculty of Science, University of M'sila, M'sila, Algeria. Email: baaziz_hakim@yahoo.fr.

21. "Evaluation of ground water quality using water quality index in Kathmandu valley, Nepal"

Dr. Tista Prasai Joshi, Senior Women Scientist, Nepal Academy of Science and Technology (NAST), Kathmandu, Nepal. Email: tistaprasai@gmail.com

22. "Optimized of tunable halide perovskites CsNX₃ as promising renewable materials for future designing of photovoltaics technologies"

Dr. M. Musa Saad H.-E., Associate Professor, Qassim University, Al-Muthnib 51931, Saudi Arabia.
Email: 141261@qu.edu.sa

23. "DFT Calculations of structural, mechanical and thermodynamic properties of nitride and carbide of Ti-Os intermetallic compounds"

Prof. Habib Rached, Professor, Hassiba Benbouali university of Chlef, Faculty of exact sciences and Informatics, Department of physics, Algeria. Email: habib_rached@yahoo.fr

Schedule:

✧ Thematic issue submission deadline:

1st June 2022

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