



Session III: Theoretical and Computational Science (TCS)

- Venue : Auditorium, Atomic Energy Centre, Dhaka
- Time : 14:00 - 15.30
- Chair(s) : Prof. Md. Ismail Jabiullah, PhD
Dept. of Computer Science and Engineering
Independent University of Bangladesh
- : Abu Zafur Ziauddin Ahmed, PhD
Assistant Professor and Chairman
Dept. of Physical & Mathematical Sciences, Primeasia University, Dhaka
- Invited Lecture : **Electronic Band Structure and the Electronic Ground States of Solids**
IL-02
Prof. Saleh Hasan Nakib, PhD
Dept. of Physics, University of Rajsahi

Contributory Papers:

Abstract ID	Title	Author Name(s)
TCS01-033	Wide-Bandgap Double Perovskites Rb ₂ KScCl ₆ and Rb ₂ NaYCl ₆ for UV Optoelectronic Applications: A First-Principles Study	Md. Al Mubin Hossain, Nayeemur Rahman, and Mohammad Abdur Rashid
TCS02-053	A DFT and SCAPS 1D Modelling Devices of Novel Double Perovskite Halides (Tl ₂ AgAsX ₆ ; X = Cl, I) for Energy Conversion Approaches	R. M. Tanvir, Md. Al-Amin, A. Rayhan, and S. Mahmud
TCS03-077	Electronic, Optical, and Various Physical Properties of Half-metallic Ferromagnetism βVO ₃ (β = Y, La): A DFT Insights	M. E. Haque Akonda, S. Karmakar, A. Ghosh, M. A. Hasan, and M. M. Rahaman
TCS04-138	First-Principles Study of Mixed-Halide Perovskites RbSrBr _{3-x} I _x : Tuning Physical Properties through Halide Alloying	Mst. Tanjum Islam, Ratna Saha, and Rinku Majumder
TCS05-238	Substituent Effects on O–H Bond Dissociation Energy in Phenolic Antioxidants: A DFT Approach	Jewel Hossen, Shahriar Siam, Md. Forhad Babu, Tanu Dey, Md. Mazharul Islam, Md. Masum Iqbal, Apel Mahamud Rabby, and Md. Tanvir Rashid Rezvi
TCS06-252	DFT Study of Safe Methotrexate Delivery Using Pristine and Heteroatom-Doped Fullerene Nanocages for Cancer Therapy	M. Rejaul Karim and A. K. M. Akther Hossain
TCS07-256	Mechanisms of Light-Ion-Induced Nuclear Reactions: A Comparative Study Using INC and TALYS	Monira Jannatul Kobra