International e-Conference on Physics 2021

9 – 11 July 2021 (Online Platform Zoom)

Theme: Glorious 100 Years of Physics in Dhaka University

Programme and Abstracts

Organized

by

Department of Physics

University of Dhaka

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CONTENTS

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PROGRAMME

Date: 9 – 11 July 2021 (Friday to Sunday)

Venue: Online Platform Zoom

Day 1, Friday, 9th July 2021 Time: 16:00 – 23:30 BST (Bangladesh Standard Time)	
Inaugural Session, 16:00-16:50 BST **Venue (Virtual, Zoom Link):** https://bdren.zoom.us/j/9829750569	
16:00-16:05	Welcome Address by the President, Organizing Committee: **Prof. Dr. A. B. M. Obaidul Islam** *Chairman, Department of Physics, University of Dhaka, Bangladesh*
16:05-16:15	Address by the Special Guest: **Prof. Dr. Md. Abdus Samad** *Dean (Acting), Faculty of Science, University of Dhaka, Bangladesh*
16:15-16:30	Address by the Guest of Honor: **Prof. Dr. A. S. M. Maksud Kamal** *Pro-Vice Chancellor (Academic), University of Dhaka, Bangladesh*
16:30-16:45	Address by the Chief Guest: **Prof. Dr. Md. Akhtaruzzaman** *Vice Chancellor, University of Dhaka, Bangladesh*
16:45-16:50	Vote of Thanks by the Secretary, Organizing Committee: **Prof. Dr. Md. Wahadoszamen** *Department of Physics, University of Dhaka, Bangladesh*
Technical Sessions	
Session-I: Keynote Session followed by an Invited Talk **Time: 17:30-19:00 BST** **Venue (Virtual, Zoom Link):** https://bdren.zoom.us/j/9829750569	
Keynote Speech	
17:30-18:25	The Photon Chasers; **Mohammad Ataul Karim**
Invited Speech	
18:25-19:00	The Opacity Project and the Iron Project: The Leap in Understanding the Astronomical Objects; **Sultana N. Nahar**

Session-II: Optics, Photonics, Laser & Ultrafast Physics (OPLUP) **Time: 19:00-21:11 BST** **Venue (Virtual, Zoom Link):** https://bdren.zoom.us/j/9829750569 **Session Chair: Prof. Dr. Aminul I. Talukder** **Session Co-chair: Dr. Zulfiqar Hasan Khan**		
Invited Talk		
19:00-19:35	**IT-II**	Laser Physics Research in the Dhaka University: Laser Spectroscopy and Laser-Ablated Nanoparticle Fabrication; **A.F.M. Yusuf Haider**
Contributory Talks		
19:35-19:47	**OPLUP-01**	Ultrafast Laser Material Processing for Industrial Applications; **Arifur Rahaman, Aravinda Kar, and Xiaoming Yu**
19:47-19:59	**OPLUP-02**	Development of Ultrahigh-Resolution Fiber-Optic Strain Sensors with Off-the-Shelf Components; **Nabil Md Rakinul Hoque, Lingze Duan**
19:59-20:11	**OPLUP-03**	Integration of Multi-layer Black Phosphorus into Photoconductive Antennas for THz Emission; **M. Hasan Doha, J. I. Santos Batista, Ahmad F. Rawwagah, Josh P. Thompson, Arash Fereidouni, Kenji Watanabe, Takashi Taniguchi, Magda O. El-Shenawee, and Hugh O. H. Churchill**
20:11-20:23	**OPLUP-04**	The Photochemistry of cis-Stilbene Studied by Ultrafast Electron Diffraction; **S. K. Saha, J. P. F. Nunes, H. Weir, B. Moore, M. Williams, A. R. Attar, D. Luo, F. Ji, M. C. Hoffmann, J. Yang, M. Lin, M. R. Ware, R. K. Jobe, S. Pathak, T. J. A. Wolf, T. J. Martinez, and M. Centurion**
20:23-20:35	**OPLUP-05**	Tracking Ultrafast Formation of Energetic Intermediates During a Photoinduced Reaction on a Particularly Disordered Surface; **Md Afjal Khan Pathan, Aakash Gupta, and Mihai E. Vaida**
20:35-20:47	**OPLUP-06**	Intervalence Band Absorption Loss Calculations of Tensile Germanium Waveguide Lasers with SiNx Stress Liners:; **Md. Shamim Reza, Istvan Gulyas, Mark A. Wistey**

20:47-20:59	**OPLUP-07**	Electron-Electron Correlations and Ultrafast Nonlinear Optical Response in Solids; **D. Alam, N. Ud Din, S. Gholam-Mirzaeimoghadar, M. Chini, V. Turkowski**
20:59-21:11	**OPLUP-08**	Design and Investigation of Polymer Multimode Interference based Waveguide Splitters for Photonic Integrated Circuits; **N. Afsary, M.N. Sakib, M.K. Alam, M.O.F. Rasel and T. Ishigure**
Session-III: Magnetic Materials & Material Science (MMMS) **Time: 21:15-23:30 BST** **Venue (Virtual, Zoom Link):** https://bdren.zoom.us/j/9829750569 **Session Chair: Prof. Dr. A K M Akther Hossian** **Session Co-chair: Dr. Kazi Hanium Maria**		
Invited Talk		
21:15-21:50	**IT-III**	Extraordinary Electrical, Optical, And Thermal Properties of Atomically Thin Two-Dimensional Crystals; **AKM Newaz**
Contributory Talks		
21:50-22:02	**MMMS-01**	High Temperature Magnetization and Lage Topological Hall Effect in Layered Materials; **Md Rafique Un Nabi, Aaron Wegner, Rabindra Basnet, Krishna Pandey, Gokul Acharya, Jin Hu**
22:02-22:14	**MMMS-02**	Study on Hydrogen Isotopes Behavior in Proton Conducting Zirconates; **M. Khalid Hossain, Kenichi Hashizume**
22:14-22:26	**MMMS-03**	Temperature Effect on Magnetization Reversal of a Magnetic Nanoparticle Driven by a Down-Chirp Microwave Field Pulse; **M. A. J. Pikul, M. A. S. Akanda, Z. K. Juthy, M.T. Islam and X. S. Wang**
22:26-22:38	**MMMS-04**	A Strategy of Swift Magnetization Reversal of Single Domain Magnetic Nanoparticle; **M. A. S. Akanda, M. A. J. Pikul, Z. K. Juthy, M.T. Islam and X. S. Wang**
22:38-22:50	**MMMS-05**	Theoretical and Experimental Investigation of Structural, Electrical and Magnetic Properties for La Substituted Ni-Cu-Cd Magnetic Ceramics Synthesize from Nanocrystalline Powders;

		M. Faishal Mahmood and M. Belal Hossen
22:50-23:02	**MMMS-06**	Effect of Yttrium on Magnetic and Electrical properties of Neodymium Ferrite Nanoparticles; **Shovan Kumar Kundu, Dhiraj Kumar Rana, Soumen Basu**
23:02-23:14	**MMMS-07**	Surface Morphological, Structural and Optical Properties of Plasma Polymerized 1,2-Diaminocyclohexane Thin Films; **Md. Mahmud Hasan, Mohammad Jellur Rahman, Md. Masud Reza, Md. Juel Sarder and A. H. Bhuiyan**
23:14-23:26	**MMMS-08**	Thermal and Optical Properties of As-deposited Plasma Polymerized N-benzylaniline Thin Films; **Rani Nasrin, Mohammad Jellur Rahman, A. T. M. K. Jamil, and A. H. Bhuiyan**
Day 2, Saturday, 10th July 2021 **Time: 19:00 – 23:30 BST (Bangladesh Standard Time)**		
Session-IV: Biophysics, Medical & Heath Physics (BMHP) **Time: 19:00-21:11 BST** **Venue (Virtual, Zoom Link):** https://bdren.zoom.us/j/9829750569 **Session Chair: Prof. Dr. Md. Wahadoszamen** **Session Co-chair: Dr. Muhammad Abdul Kadir**		
Invited Talk		
19:00-19:35	IT-IV	The Quantum Design of Photosynthesis; **Rienk van Grondelle**
Contributory Talks		
19:35-19:47	**BMHP-01**	Promising Gradient Waveforms for FRONSAC Encoding for Clinical Brain Imaging; **E. H. Bhuiyan, R. T. Constable, G. Galiana**
19:47-19:59	**BMHP-02**	Single Molecule Investigation of Tandem G-Quadruplex Structures Formed by Human Telomeric Sequence; **Golam Mustafa, Sajad Sheikh, Keshav GC, Sanjaya Abeysirigunawardena, Hamza Balci**
19:59-20:11	**BMHP-03**	DLSCORE: A Deep Learning Model for Predicting Protein-Ligand Binding Affinities; **Md Mahmudulla Hassan, Daniel Castañeda Mogollón, Olac Fuentes, and Suman Sirimulla**

20:11-20:23	**BMHP-04**	Theoretical Investigation on The Feasibility of Dual Energy X-Ray Imaging of Chronic Obstructive Pulmonary Disease; **Fateen Basharat, Michael Belli, Miranda Kirby, and Jesse Tanguay**
20:23-20:35	**BMHP-05**	Pore Size Dependent Molecular Transport to Guvs using COMSOL Simulation; **Md. K. Alam, T. Rahman, M. S. Ishtiaque, M. I. Hossain, and M.A.S. Karal**
20:35-20:47	**BMHP-06**	Continuous Radiation Monitoring at Atomic Energy Centre Dhaka Campus using Thermoluminescent Dosimeters; **Avijit Biswas, M. S. Rahman, S. Yeasmin, and Md. Kabir Uddin Sikder**
20:47-20:59	**BMHP-07**	Real-time Indoor Radiation Monitoring at INMAS Mitford Hospital Campus following In-Situ Method and Estimation of Radiological Risk on Worker & Public; **L. A. Tonu, M. S. Rahman, Pretam K. Das, and S. Yeasmin**
20:59-21:11	**BMHP-08**	Spatial Distribution and Contamination of Trace Elements in Surface Sediments of the Kaptai Lake, Bangladesh using Neutron Activation Analysis; **Biplob Das, Mohammad Amirul Islam, Umma Tamim, Rahat Khan, and Mohammad Belal Hossen**
Session-V: Theoretical Condensed Matter Physics (TCMP)-I **Time: 21:15-23:15 BST** **Venue (Virtual, Zoom Link):** https://bdren.zoom.us/j/9829750569 **Session Chair: Prof. Dr. Golam Mohammed Bhuiyan** **Session Co-chair: Dr. Alamgir Kair**		
Invited Talk		
21:15-21:50	**IT-V**	Tuning Properties of Two-Dimensional Materials for a Sustainable Future; **Talat S. Rahman**
Contributory Talks		
21:50-22:02	**TCMP-01**	Multiple Superexchange Interactions for Ferromagnetic Insulator in Rare Earth Oxides; **Md Mokhlesur Rahman and Jaichan Lee**
22:02-22:14	**TCMP-02**	The Adsorption of Oxygen on Bimetallic Pd_3M_2 Clusters (M =

		Ag, Au, Co, Cu, Mn, Ni, Pt and Ru) with and without Alumina Support by Density Functional Theory; **Nusaiba Zaman, Kah Chun Lau, Abdelkader Kara**
22:14-22:26	**TCMP-03**	A First-principles Investigation of Physical Properties of Topological Weyl Semimetals Ta*X* (*X* = P, As); **M. I. Naher and S. H. Naqib**
22:26-22:38	**TCMP-04**	DFT+U Study of the Structural, Magnetic and Optical Properties of Pure and (Fe, Co) Co-doped CuO Nanoparticles; **Mainul Abrar, Sadiq Shahriyar Nishat, and Alamgir Kabir**
22:38-22:50	**TCMP-05**	Calculation of Electrical Resistivity for Liquid Binary Cu_xAg_{1-x} Alloys; **Asma Harun and R.C. Gosh**
22:50-23:02	**TCMP-06**	Density Functional Study of Pressure Dependent Physical Properties of SnS and Sb_2S_3; **Ayesha Tasnim, Md. Mahamudujjaman, R. S. Islam, and S. H. Naqib**
23:02-23:14	**TCMP-07**	A DFT with Advanced Functionals (DFT+U) Study of Cubic and Hexagonal ZnX (X= O, S, Se, Te) for Potential Optoelectronic Device Application; **Eashika Mahmud, Sarker Md. Sadman, Muhammad Rakibul Islam**
Day 3, Sunday, 11th July 2021 **Time: 19:00 – 23:30 BST (Bangladesh Standard Time)**		
Session-VI: Experimental Condensed Matter Physics (ECMP) **Time: 19:00-21:11 BST** **Venue (Virtual, Zoom Link):** https://bdren.zoom.us/j/9829750569 **Session Chair: Prof. Dr. A B M Obaidul Islam** **Session Co-chair: Dr. Mahabub Alam Bhuiyan**		
Invited Talk		
19:00-19:35	**IT-VI**	Band Structure Engineering and Heterojunction of Two-dimensional Transition Metal Dichalcogenides; **Saiful I. Khondaker**
Contributory Talks		
19:35-19:47	**ECMP-01**	Improved Electrical Properties of *in-situ* SiNx Passivated AlGaN/GaN HEMT by Tailoring the Stoichiometry of the Passivated Layer; **Anwar Siddique, Raju Ahmed, Jonathan**

		Anderson, Mark Holtz, and Edwin L. Piner
19:47-19:59	**ECMP -02**	Drastic Enhancement of Efficiency in DSSC by Electrosorption; **Ganapathi Rao Kandregula, Jagadeeswari Sivanadanam, and Kothandaraman Ramanujam**
19:59-20:11	**ECMP -03**	Electron Transport in Photochromic Rare-earth Metal Oxy-hydride Thin Films; **S. Kazi, D. Moldarev, M. V. Moro, D. Primetzhofer, M. Wolff**
20:11-20:23	**ECMP -04**	Studies on Dielectric and Photocatalytic Properties of Zeolite/MWCNT Nanocomposite; **Shwetha S, Jithin P. V., Rakesh K. E., Deepu Thomas**
20:23-20:35	**ECMP -05**	Synthesis and Characterization of GO Based PVA Nanocomposites Based on GO using Reduced Percentage of GO Nanofillers; **Md. Wahidujjaman Bari, K.M. Abu Hurayra–Lizu, Muhammad Rakibul Islam**
20:35-20:47	**ECMP -06**	Thickness Dependent Optical Properties of the AC Plasma Polymerized 3,4-Ethylenedioxythiophene Thin Films; **Md. Juel Sarder, Mohammad Jellur Rahman, Md. Mahmud Hasan, and A. H. Bhuiyan**
20:47-20:59	**ECMP -07**	Wide Bandgap Ga_2O_3 Based Alloy by Pulsed Laser Deposition; **Md Dalim Mia, Brian Samuels, Ahad Talukder and Ravi Droopad**
20:59-21:11	**ECMP -08**	MBE Growth of High-Quality GaAs on C-plane Sapphire Substrate; **Samir K. Saha, R. Kumar, Andrian Kuchuk, Yurii Maidaniuk, Yuriy I. Mazur, Shui-Qing Yu, and G. J. Salamo**
Session-VII: Theoretical Condensed Matter Physics (TCMP)-II **Time: 21:15-23:15 BST** **Venue (Virtual, Zoom Link):** https://bdren.zoom.us/j/9829750569 **Session Chair: Prof. Dr. Ishtiaque M. Syed** **Session Co-chair: Dr. Ratan Chandra Gosh**		
Invited Talk		
21:15-21:50	**IT-VII**	Bosons in High-T_c Cuprates: Where Do We Stand?; **S. H. Naqib and R. S. Islam**

Contributory Talks		
21:50-22:02	**TCMP-08**	Effect of Dilute Magnetism in a Topological Insulator; **Firoza Kabir, M. Mofazzel Hosen, Xiaxin Ding, Christopher Lane, Gyanendra Dhakal, Yangyang Liu, Klauss Dimitri, Christopher Sims, Sabin Regmi, Anup Pradhan Sakhya, Luis Persaud, John E Beetar, Yong Liu, Michael Chini, Arjun K. Pathak, Jian-Xin Zhu, Krzysztof Gofryk, and Madhab Neupane**
22:02-22:14	**TCMP-09**	Fermi Surface Mapping of Non-Trivial Topological Semimetal Candidate $CaSn_3$; **K A M Hasan Siddiquee, Riffat Munir, Charuni Dissanayake, Xinzhe Hu, Swapnil Yadav, Yasumasa Takano, Eun Sang Choi, Talat S Rahman, Duy Le, and Yasuyuki Nakajima**
22:14-22:26	**TCMP-10**	Search for a Light Pseudoscalar Higgs Boson in the Two Higgs Doublet Model using Data from the Large Hadron Collider (LHC); **Maxwell Chertok, Jack Gunion, Redwan Md Habibullah, Grace Haza, Rachel Yohay, Fengwangdong Zhang, Jingyu Zhang**
22:26-22:38	**TCMP-11**	Justification of the Scaling Law of Dzugutov for Diffusion Coefficients of Liquid $Cu_xAg_{(1-x)}$ Alloys; **P. Paul and R.C. Gosh**
22:38-22:50	**TCMP-12**	Experimental and First Principles Look into $BiVO_4$; **Jannatul Fardush Tanha, U. Honey, N. I. Tanvir, Tarique Hasan, Sadiq Shahriyar Nishat, Alamgir Kabir, Shahran Ahmed, M. N. I. Khan, Md. Saiful Quddus, Imtiaz Ahmed, and S. F. U. Farhad**
22:50-23:02	**TCMP-13**	A Theoretical Based Study on Atomic Transport Properties of Liquid Simple Metals; **Mahir Manna and R.C. Gosh**
23:02-23:14	**TCMP-14**	Physical Properties of Transition Metal Dichalcogenides ZrX_2 (X = S, Se, Te): First-principles Insights; **Md. Mahamudujjaman, Md. Asif Afzal, R. S. Islam, and S. H. Naqib**
23:15-23:30	**Closing Speech**	Secretary, Organizing Committee: **Prof. Dr. Md. Wahadoszamen**

Invited Speakers List

Sl. No.	Session Name	Session Number	Invited Speaker
1.	Keynote Session followed by an Invited Talk	I	Mohammad Ataul Karim, Ph.D. Sultana N. Nahar, Ph.D.
2.	Optics, Photonics, Laser & Ultrafast Physics	II	A F M Yusuf Haider, Ph.D.
3.	Magnetic Materials & Material Science	III	A K M Newaz, Ph.D.
4.	Biophysics, Medical & Heath Physics	IV	Rienk van Grondelle, Ph.D.
5.	Theoretical Condensed Matter Physics-I	V	Talat S. Rahman, Ph.D.
6.	Experimental Condensed Matter Physics	VI	Saiful I. Khondaker, Ph.D.
7.	Theoretical Condensed Matter Physics-II	VII	S. H. Naqib, Ph.D.

Session Chairs & Co-Chairs List

Sl. No.	Session Name	Session Number	Chairs & Co-Chairs
1.	Keynote	I	Prof. Dr. A. B. M. Obaidul Islam
2.	Optics, Photonics, Laser & Ultrafast Physics	II	Prof. Dr. Aminul I. Talukder (Chair) Dr. Zulfiqar Hasan Khan (Co-Chair)
3.	Magnetic Materials & Material Science	III	Prof. Dr. A K M Akther Hossian (Chair) Dr. Kazi Hanium Maria (Co-Chair)
4.	Biophysics, Medical & Heath Physics	IV	Prof. Dr. Md. Wahadoszamen (Chair) Dr. Muhammad Abdul Kadir (Co-Chair)
5.	Theoretical Condensed Matter Physics-I	V	Prof. Dr. Golam Mohammed Bhuiyan (Chair) Dr. Alamgir Kair (Co-Chair)
6.	Experimental Condensed Matter Physics	VI	Prof. Dr. A. B. M. Obaidul Islam (Chair) Dr. Mahabub Alam Bhuiyan (Co-Chair)
7.	Theoretical Condensed Matter Physics-II	VII	Prof. Dr. Ishtiaque M. Syed (Chair) Dr. Ratan Chandra Gosh (Co-Chair)

ABSTRACTS

Session-I

Keynote Session followed by an Invited Talk

Keynote Speech

THE PHOTON CHASERS

Mohammad Ataul Karim

Professor, Electrical and Computer Engineering
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The earliest use of light as signal or in communication can be traced to use of mirrors, fire beacons, and smoke signals. This presentation will highlight and describe major milestones leading up to 12th century that contributed to the evolution of both geometrical and physical optics and how this affected our current understanding of astronomy, coherence, and signal transmission. The major players behind this maturation of photonics, who had lived and worked in areas that now lies in China, Egypt, Greece, Iraq, Iran, Spain, and Syria, will be discussed along with their works and discoveries in chronological order. The speaker will show that this process, that relied once only on philosophical discourses culminated in both experimentation and analysis, was a function of concurrent evolution of number systems, algebra, and analytical geometry.

[1]. David C. Lindberg, The Beginnings of Western Science, University of Chicago Press, 2007.
[2]. Bradley Steffens, Ibn Al-Haytham: First Scientist, Morgan Reynolds Publishing, 2007.

Invited Speech

The Opacity Project and the Iron Project: The Leap in Understanding the Astronomical Objects

Sultana N. Nahar

Department of Astronomy, The Ohio State University, Columbus, OH 43210, USA

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The two international collaborations, the Opacity Project (OP) and the Iron Project (IP), have brought a leap in understanding the astronomical objects, such as, interpretation of their physical conditions and chemical evolutions, photo-absorption and radiation transport, abundances of elements, temperature and pressure diagnostics, the spectral analysis of emission and absorption of radiation, etc. The underlying science has been finding the characteristic features of radiative and collisional atomic processes in astrophysical plasmas. These require quite of number of scientific investigators, development of theories and extensive codes based on R-matrix methodologies, and availability of high performance super computers. The effort has resulted in solving a number of long standing problems, finding new atomic features and creation of four atomic databases, as an active member of the OP and the IP, I will summarize some of our current understandings and future direction.

Session-II

Optics, Photonics, Laser & Ultrafast Physics (OPLUP)

Invited Talk

IT-II: Laser Physics Research in The Dhaka University: Laser Spectroscopy and Laser-Ablated Nanoparticle Fabrication

A.F.M. Yusuf Haider[1,2]

[1]*Physics Department, University of Dhaka, Dhaka, Bangladesh.*
[2]*Present affiliation: Department of Mathematics and Natural Sciences, BRAC University, Bangladesh.*

Email: yusuf.haider@bracu.ac.bd

The study of laser physics started in the physics department in the year 1984 and in fact for the first time in Bangladesh, with the introduction of a course on laser physics at the postgraduate level and with the establishment of a research laboratory in the department. Finally, it culminated in an excellent laboratory on laser physics with the establishment of a Non-linear optics and laser spectroscopy laboratory at the Center of Advanced Research in Science (CARS). CARS was established at the initiative of the author when he was the pro-vice-chancellor of Dhaka University.

In this talk, the principles and the applications of Laser-induced Breakdown Spectroscopy (LIBS), Laser Raman Spectroscopy (LSR), and laser fabrication of nanoparticles will be discussed. The LIBS applications on elemental analyses, detection of trace amount of toxic elements in materials at sub-ppm level, lifetime measurements of atoms in gaseous states and diagnostics of the micro-plasma produced by the higher power laser pulse will be discussed. LRS application in determining the level of saturation/unsaturation of fatty acids in edible oils will also be presented. Finally, the fabrication and morphological studies of gold and silver nanoparticles produced by high-power laser pulses will be presented.

Contributory Talks

OPLUP-01: Ultrafast Laser Material Processing for Industrial Applications

Arifur Rahaman*, Aravinda Kar, and Xiaoming Yu

CREOL, The College of Optics & Photonics, University of Central Florida, Orlando, Florida 32816, USA.

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Ultrafast laser has been used for high precision material processing since it was invented. Due to its unique characteristics and capability, ultrafast laser can be used to modify almost all materials and enabling various applications ranging from micromachining, photonics to life sciences. However, there are challenges when this technology is applying in industrial applications, which require scale and throughput different from lab use. To make ultrafast laser materials processing compatible for industrial applications, it is a common practice to run the laser at a high repetition rate and hence high average power. However, heat accumulation under such processing conditions will deteriorate processing quality, especially for polymers, which typically have a low melting temperature. In this talk, I will present engineering techniques that overcome these challenges to apply ultrafast laser for industrial and scientific applications.

OPLUP-02: Development of Ultrahigh-Resolution Fiber-Optic Strain Sensors with Off-the-Shelf Components

Nabil Md Rakinul Hoque*, Lingze Duan

Department of Physics and Astronomy, The University of Alabama in Huntsville, USA

*Email: nh0014@uah.edu

Over the last three decades, fiber-optic sensing has grown into a major sector in the sensing industry with its broad applications in various fields including aerospace engineering, civil engineering, oil/gas exploration, homeland security, geophysics, biomedicine etc. Fiber-optic sensors offer numerous advantages over other types of sensors, such as high sensitivity, high flexibility, lightweight and compactness, environmental ruggedness, and immunity to electromagnetic interference. Considering these facts, here we present the development of an ultrasensitive fiber-optic sensor based on only off-the-shelf components. In this scheme, a meter-long fiber Fabry-Perot interferometer (FFPI) with a finesse of ~1000 is used to probe tiny strain signals. The sharp spectral feature of its resonance peaks allows the FFPI to achieve a very high strain resolution. There are, however, some practical challenges associated with reliably interrogating the FFPI. These challenges are addressed by introducing adequate insulation through a fiberglass box, sound-absorbing foams, and a vibrational isolator. In addition, to enhance the strain resolution at low frequencies, a dual-FFPI based sensing scheme is proposed. The main advantage of this scheme lies in the fact that the environmental noise is nullified as a common-mode noise. This allows us to achieve higher strain resolutions than the previously reported best results by roughly a factor of 2 without using complicated laser frequency stabilization or expensive vacuum systems. This work paves the way for our future research on thermal-noise-limited fiber-optic sensing.

OPLUP-03: Integration of Multi-layer Black Phosphorus into Photoconductive Antennas for THz Emission

M. Hasan Doha[1,*], J. I. Santos Batista[2], Ahmad F. Rawwagah[3], Josh P. Thompson[1], Arash Fereidouni[1], Kenji Watanabe[3], Takashi Taniguchi[3], Magda O. El-Shenawee[2,5], and Hugh O. H. Churchill[1,5]

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[3]*National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan*
[4]*Department of Electrical Engineering, University of Arkansas, Fayetteville, Arkansas 72701, U.S.A.*
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In this presentation, we report the fabrication, characterization, and modeling of photoconductive antennas by using Black Phosphorus (BP; ~ 40 nm thin-film as the photoconductor) and hexagonal boron nitride (hBN; as a capping layer that prevents the oxidation of BP). BP and hBN flakes were transferred inside a nitrogen glovebox onto dipole antennas (fabricated on oxidized high-resistivity Si substrates). The thickness of the BP and hBN were optimized for maximum absorption within the BP layer using the transfer matrix method. The crystal orientation of BP flakes was determined using differential reflection anisotropy and the armchair axis was aligned with the anode-cathode gap of the antenna. Under illumination with 100 fs pulses at 780 (1560) nm, photocurrent imaging shows a bias-dependent maximum photocurrent localized to the antenna gap with a peak photoconductivity 1 (2) S/cm in the linear regime of bias [1]. Device performance was modeled numerically by solving Maxwell's and the drift-diffusion equations to obtain the photocurrent density in response to pulsed laser excitation, showing qualitative agreement with the experimental observations. These devices present a step toward high-performance THz photoconductive antennas using BP. We will also describe ongoing THz time-domain spectroscopy measurements of these devices.

[1] Doha, M. H. et al. *J. Appl. Phys*, **128**(6), 063104 (2020).

OPLUP-04: The Photochemistry of cis-Stilbene Studied by Ultrafast Electron Diffraction

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Stilbene is a model system for studying both photoisomerization and photocyclization mechanisms, commonly pivotal to the conversion of light into chemical and mechanical energy in nature. Despite multi-decades of research, the exact details of the photoisomerization of cis-stilbene into trans-stilbene and/or its

cyclization into 4a,4b-dihydrophenanthrene (DHP) have remained a topic of debate. Here we used mega-electronvolt ultrafast electron diffraction (UED) to capture and spatially resolve the photoisomerization and/or photocyclization of cis stilbene with sub-angstrom resolution and shed some light on the mechanisms mediating its rich photochemistry. At the SLAC MeV-UED beamline, cis-stilbene was optically pumped with 267 nm ultraviolet light and probed with 3.7 MeV electrons. Analyses of the difference-diffraction signals revealed features across a wide momentum transfer range, up to 8Å-1. These features were found to be in good qualitative agreement with the difference signal predicted by Ab initio multiple spawning simulations.

OPLUP-05: Tracking Ultrafast Formation of Energetic Intermediates During a Photoinduced Reaction on a Particularly Disordered Surface

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In this contribution, the ultrafast photoinduced reaction of a model system consisting of CD_3I molecules on an amorphous ceria surface is studied to understand the effect of surface morphology on the reaction dynamics. An experimental approach that combines time-of-flight mass spectrometry with pump-probe spectroscopy is employed to enable time-resolved investigation of the reaction mechanism through the detection of intermediate species and final products directly from the surface. The photoreaction of CD_3I on the ceria surface is triggered by a pump laser pulse at a central wavelength of 266 nm, which directly excites the molecule into the dissociative A-band via a single photon absorption. Subsequently, the neutral fragments on the surface, i.e., CD_3 and I, can either desorb or further react with the neighboring species to form I_2 or reform CD_3I molecule. The probe laser pulse in the UV spectral domain is used to ionize and sensitively detect the reaction intermediates and final products as a function of the pump-probe time delay. The time constants that are deduced from the transient evolution of the mass spectra signals of CD_3^+, I^+, $CD_3I^{+,}$ and I_2^+ provide insights into the adsorption geometry of the CD_3I molecules on the surface as well as the reaction dynamics. The photofragments after generation are observed to lose their kinetic energy over time through the interaction with the substrate and neighboring species, thermalize, and eventually react to each other to form I_2 and reform CD_3I.

OPLUP-06: Intervalence Band Absorption Loss Calculations of Tensile Germanium Waveguide Lasers with SiNx Stress Liners

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Germanium (Ge) is long being considered as a potential candidate for a group IV-based photonics material because of its nearly direct bandgap. In Ge, the conduction band (CB) direct valley (k = 0) is normally 140 meV above the indirect valley. However, tensile strains of 1.9% (biaxial) or 4% (uniaxial) transform Ge into a

direct bandgap material suitable for lasers and active gain regions [1]. Though several research groups have shown optical emission from strained Ge, the devices required very high threshold current density to operate, and their efficiency was very low. In this work, we used ab-initio and finite element strain modeling to explain high threshold current densities in a strained Ge waveguide laser. We found that, anisotropic strains improve carrier confinement but reduce the optical confinement, and intervalence band absorption (IVBA) still dominates. For a carrier injection of $\Delta n = \Delta p = 1.25\,x\,10^{19}\,cm^{-3}$ with anisotropic biaxial tensile strain and n^{++} doping, the maximum reported IVBA is $2740\,cm^{-1}$. Finally, we conclude at higher biaxial tensile strain and n^{++} doping, it is possible to make a CMOS compatible laser, but further reducing the direct bandgap by adding Sn or C would vastly improve threshold currents.

[1] J. Liu, L. C. Kimerling, and J. Michel, Monolithic Ge-on-Si lasers for large-scale electronic–photonic integration, *Semiconductor Science Technology*, **27**(9), p. 094006, (2012).

OPLUP-07: Electron-Electron Correlations and Ultrafast Nonlinear Optical Response in Solids

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The interaction of electrons in solid with a strong laser-pulse field introduces many interesting phenomena. One of the compelling effects is the high harmonic generation (HHG)- nonperturbative emission of light with frequencies that are integers of the pulse frequency. HHG is an efficient experimental method to study the effects of the interaction of electrons with light and the electron dynamics. A significant progress has already been made in understanding of the details of the microscopic mechanism behind HHG, like the role of intra- and inter-band transitions, the contribution of the modulus, and the phase of the dipole moment to even and odd harmonic peaks, the role of the oscillating dipoles and “traditional” currents, effects of broken symmetry, etc. However, the role of electron-electron correlations, particularly for HHG in strongly-correlated materials, is much less understood. In this talk, we present result on the role of these effects in the high-harmonic (HH) spectrum of perovskite BaTiO3 obtained by using the time-dependent density-functional theory with the exchange-correlation kernel calculated with dynamical-mean field theory. As we demonstrate, the correlation effects significantly modify the HH spectrum, in particular shifting the spectrum to higher frequencies and changing the polarization direction of the harmonic emission. The results obtained may help to shed the light on the role of correlation effects in the electronic and optical properties of strongly-correlated materials.

OPLUP-08: Design and Investigation of Polymer Multimode Interference based Waveguide Splitters for Photonic Integrated Circuits

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The current dominating electronic integrated circuits consume more energy due to the skin effect. The combination of an inductor, capacitor and impedance in copper links causes high power dissipation loss. Alternatively, photonic integrated circuits (PICs) have drawn intensive attention utilizing the flow of photons through the circuits. This research demonstrates multimode interference (MMI) based waveguide splitters realized with polymer materials because the polymer waveguides exhibit high flexibility, low loss, and easy integration on printed circuit boards (PCBs). The schematic of this polymer optical MMI waveguide splitters consists of a single input and multiple outputs (five outputs), where the core diameters of the input and outputs are fixed to 6 µm, and the core spacing between the outputs is controlled to be 17 µm. The core and cladding materials for this MMI splitter are NP-005 (refractive index: 1.575 at 1550 nm) and NP-211 (refractive index: 1.567at 1550 nm), respectively. We have investigated this polymer MMI splitter by applying the commercially available beam propagation method (BPM) solver at 1550-nm wavelength and analyzed the self-imaging length of the step-index (SI) and graded-index (GI) core profiles of this polymer splitters. After a couple of investigations, the optimum self-imaging length and width of this MMI section are confirmed. The suitable length and width for the SI MMI waveguide splitter are L_{mmi}=3200 µm and W_{mmi}=85 µm, respectively, at 1550 nm. The efficiency of the intensity of this MMI splitter is approximately 76%. We also investigate the insertion loss, excess loss, uniformity of this MMI waveguide splitter.

Session-III

Magnetic Materials & Material Science (MMMS)

Invited Talk

IT-III: Extraordinary Electrical, Optical, and Thermal Properties of Atomically Thin Two-Dimensional Crystals

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Two-dimensional (2D) atomic crystals are recently discovered materials that are only atoms thick, and yet can span laterally over millimeters. The diverse family of such materials includes graphene: a semimetal with massless relativistic charge carriers, and monolayer transition metal dichalcogenides (TMDCs), such as molybdenum disulfide (MoS_2): a direct bandgap semiconductor. The fascinating thermal, electronic, optical, and chemical properties of these materials as well as their promise of new applications arising from these properties have enchanted researchers from diverse fields such as physics, chemistry, materials science, and nanotechnology. In this presentation, I will talk about the extraordinary electrical, thermal, and optical properties of 2D atomic crystals and their heterostructures, and future device applications.

[1]. Hao Lee, S. Deshmukh, Jing Wen, V.Z. Costa, J. S. Schuder, M. Sanchez, A. Ichimura, Eric Pop, Bin Wang, and A. K. M. Newaz, Layer dependent Interfacial Transport and Optoelectrical properties of MoS_2 on Ultra-flat metals- *ACS Applied Materials and Interfaces*, **11,** 31543-31550, (2019).

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Contributory Talks

MMMS-01: High Temperature Magnetization and Lage Topological Hall Effect in Layered Materials

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Mn_2Sb and MnZnSb are characterized in a Cu_2Sb-type structure but exhibit different magnetic and transport properties. Mn_2Sb is ferrimagnetic below the T_c~550K with magnetic moment aligned parallel to c-axis and undergo a spin-flip transition around 240K where the magnetic moment is aligned parallel to a-b plane. Meanwhile, MnZnSb is a at room temperature ferromagnet. We synthesized $Mn_{1+x}Zn_{1-x}Sb$ ($0 < x < 1$) single crystals and studied the evolution of magnetic and transport properties. We probed two magnetic phase transitions and observed anomalous hall effect in $Mn_{1+x}Zn_{1-x}Sb$ which changes sign with decreasing temperature. In addition, we have probed topological Hall effect likely to be attributed to spin texture. Our discoveries provide a new platform to study the tuning of magnetism and possibly offer a new 2D magnetic system.

MMMS-02: Study on Hydrogen Isotopes Behavior in Proton Conducting Zirconates

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In this study, hydrogen solubility and diffusivity behavior in three different proton-conducting oxides, $BaZr_{0.9}Y_{0.1}O_{2.95}$ (BZY), $BaZr_{0.955}Y_{0.03}Co_{0.015}O_{2.97}$ (BZYC), and $CaZr_{0.9}In_{0.1}O_{2.95}$ (CZI), were studied by the tritium imaging plate (TIP) technique using a hydrogen-tritium gas mixture (HT) (T = 0.0001%, ~1.3kPa) and also partially-tritiated heavy water vapor (DTO) (T = 0.1%, ~2kPa) in the temperature range of 623 to 1273 K. The hydrogen solubility and diffusivity behavior in BZY, BZYC, and CZI were also studied by thermal desorption spectroscopy (TDS) using deuterium (D_2), and heavy water (D_2O). The oxide specimens were prepared with conventional powder metallurgy using BZY, BZYC, and CZI powders separately by being die-pressed, cold-isostatically-pressed (200MPa), and sintered in air at 1913 K for 20 h. The specimens obtained were having a disc shape (~7.5 mm in diameter, ~2.3 mm in thickness) and more than 95% TD. From Imaging Plate (IP) images for the surface of all tritium (T) exposed specimens, uniform T distribution was found. Observing cross-sectional T-concentration profiles of cut specimens allowed us to determine hydrogen solubility and diffusivity in the specimens. In all cases of tritium exposure (HT and DTO), BZYC always shows the highest hydrogen solubility, while CZI always shows the lowest one. In DTO exposure, the BZY shows the highest hydrogen diffusivity, while in HT the BZYC shows the highest one. In all cases, CZI shows almost one order lower solubility and diffusivity than the BZY and BZYC. These results mean that barium zirconates show better electrochemical performance than the calcium zirconate and that a small amount of Y

and Co doping in $BaZrO_3$ may play a vital role in the enhancement of its electrochemical activity, which is suitable for various electrochemical devices like fuel cell, hydrogen pump, hydrogen sensor, etc., and also for tritium purification and recovery system in nuclear fusion reactors.

MMMS-03: Temperature Effect on Magnetization Reversal of a Magnetic Nanoparticle Driven by a Down-chirp Microwave Field Pulse

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It has been shown that a single-domain magnetic nanoparticle can be effectively switched by a linear down-chirp microwave field pulse (DCMWP) in zero temperature limit. However, finite temperature is ubiquitous in practice. Here, we study the effect of finite temperature on the DCMWP-induced magnetization reversal based on the stochastic Landau-Lifshitz-Gilbert equation. It is found that any one of the three controlling parameters of a DCMWP, i.e. the amplitude, chirp rate, or initial frequency, decreases with increasing temperature while the other two are fixed. The maximal temperature at which the reversal can happen increases with enlarging the system size. These phenomena are related to the facts that the energy barrier induced by anisotropy increases with the system volume, and the effective magnetization decreases with temperature. We also provide a set of optimal parameters for practical realization of our proposal. These findings may provide a way to realize low-cost and fast magnetization reversal with a wide operating temperature.

MMMS-04: A Strategy of Swift Magnetization Reversal of Single Domain Magnetic Nanoparticle

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We investigate the magnetization reversal of single-domain magnetic nanoparticles driven by the circularly polarized cosine chirp microwave pulse (CCMWP). The numerical findings, based on the Landau-Lifshitz-Gilbert equation, reveal that the CCMWP can induce fast and energy-efficient magnetization reversal since the required parameters of a CCMWP, i.e., the microwave field amplitude, initial frequency, and chirp rate are much smaller than that of the linear down chirp microwave pulse (LDCMWP). This is obtained as the frequency change of the CCMWP closely matches the frequency change of the magnetization precession which leads to an efficient stimulated microwave energy absorption (emission) by (from) the magnetic particle before (after) it crosses over the energy barrier. Moreover, we found that the enhancement of the shape anisotropy field significantly reduces the required microwave amplitude and the initial frequency of CCMWP. And materials with larger damping are better for fast magnetization reversal. The investigations may give a pathway to realize the fast and low-cost memory device.

MMMS-05: Theoretical and Experimental Investigation of Structural, Electrical and Magnetic Properties for La Substituted Ni-Cu-Cd Magnetic Ceramics Synthesize from Nanocrystalline Powders

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$Ni_{0.5}Cu_{0.2}Cd_{0.3}La_xFe_{2-x}O_4$ ceramics were prepared from sol-gel synthesize nanoparticles and sintered at 1200 ºC for 5 hr. Using the sintered specimen at room temperature, the structural properties along with Rietveld refinement, magnetic, dielectric and electrical transport properties have been analyzed. The structural analysis is performed through XRD as well as Rietveld refinement to analyze the crystal phase formation. Frequency dependent complex dielectric constant show usual nature of magnetic ceramics and fitted by non-modified Debye equation. The variation of dielectric loss tangent has been analyzed and it is depicted that it reduces remarkably with increasing La content. Electric modulus analysis of the studied samples provides the information about the dynamics of conduction mechanism of the ceramics. In addition of dielectric analysis, impedance spectroscopy measurements are performed for studying the impedance nature and the measured data are also fitted to the well-known Cole-Cole plot. The usual nature of grain and grain boundary resistive and capacitive contribution has been found in the characteristics of electrical impedance. The influence of La^{3+} substitution on the magnetic permeability spectrum of the sample is studied at room temperature. The real part of permeability spectrum had been observed frequency independent nature and shows a better quality factor with La content. It has been seen that the samples exhibit ferromagnetic behavior at room temperature obtained from the magnetic hysteresis and law of approach to saturation used to determine various hysteresis parameters. There are strong correlation between dielectric loss tangent and the magnetic Q-factor at the optimum frequency band. The applicability of this compound for high frequency appliances is analyzed through this research.

MMMS-06: Effect of Yttrium on Magnetic and Electrical properties of Neodymium Ferrite nanoparticles

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The materials having multifunctional characteristics are considered as the principal base materials in multifunctional and nano-dimensional devices industries. Multiferroics are the combination of more than one ferroic characteristics (ferroelectric, ferromagnetic/antiferromagnetic and often ferroelastic) in the same phase. There is a coupling between spontaneous polarization and large magnetization. Research interest in multiferroic has increased in recent days because of their potential application in microelectronic and nano-electronic devices like transducers, spintronics, sensors, actuators. Interestingly, it was found that Neodymium Ferrite ($NdFeO_3$), a member of the centrosymmetric rare earth ortho-ferrite ($RFeO_3$) family (having a distorted

orthorhombic perovskite structure), possesses magnetically tunable ferroelectricity due to the exchange striction mechanism.

The structural properties are analyzed by XRD pattern using Rietveld refinement. TEM images confirm that average particle decreases from 70 nm to 54 nm. The DC and AC charge transport mechanism are analyzed, and the experimental data is well supported with the theoretical model, i.e. Mott's VRH model, and CBH model. M-H hysteresis loops reveal the antiferromagnetic ordering of the samples. Positive magneto-dielectric coupling is observed in the samples where coupling increases with doping which states that the Y doped $NdFeO_3$ can be good candidate in in magneto-electric industries.

MMMS-07: Surface Morphological, Structural and Optical Properties of Plasma Polymerized 1,2-Diaminocyclohexane Thin Films

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Plasma polymerized 1,2-diaminocyclohexene (PPDACH) thin films of varying thicknesses were fabricated onto ultrasonically cleaned glass substrates at room temperature by using capacitively coupled parallel plate low-pressure glow discharge RF plasma. The prepared films have been characterized by FESEM, UV-Visible and FT-IR spectroscopies, to investigate the surface morphological, optical, and structural properties, respectively. Smooth, homogenous and pinhole free surfaces of the films are confirmed by FESEM micrographs. The compositional elements of the films have been confirmed by EDX. From EDX analyses, it is observed that the prominent percentage of carbon (C), nitrogen (N) and small percentage of oxygen (O) are present in the PPDACH thin films. The FTIR results substantiate the conclusion that the plasma polymerization process modifies the structure of the polymer considerably from the monomer structure. The NH_2 group of the monomer was converted into [-NH-NH-] polymer bond, which is an indication of degradation or reorganization of monomer molecules during plasma polymerization. From UV-Visible absorption spectra, the values of direct optical transition energies (optical band gap ($E_{g(d)}$) of the films are found to be nearly equal (~ 4.04 eV). On the other hand, the indirect band gaps ($E_{g(i)}$) decrease from 2.78 – 2.58 eV with increasing film thickness. Thus PPDACH films would be suitable for different types of optoelectronic devices.

MMMS-08: Thermal and Optical Properties of As-deposited Plasma Polymerized N-benzylaniline Thin Films

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The plasma polymerized N-benzylaniline (PPNBA) thin films of different thicknesses are deposited onto glass substrates at room temperature by a parallel plate capacitively coupled AC (f = 50 Hz) plasma system using N-benzylaniline (NBA) precursor. It is observed that the as-deposited PPNBA thin films are thermally stable, the stability increases with film thickness, d and are stable up to 640 K for higher thickness film. Optical properties of the as-deposited PPNBA thin films, taken from UV-Vis spectroscopy, reveal that the absorbance is increased and broadened with the increase of d due to the π–π^* transition. The changes of optical band gap as a function of d are related to the extent of conjugation between adjacent rings of quinoid and benzenoid units in PPNBA thin films. The Urbach energy of the film decreases from 0.63 to 0.56 eV and the steepness parameter changes from 0.041 to 0.045 with the increase of d. At 325 nm, the values of extinction coefficient are found to be as small as 0.124–0.152 and those of refractive index values are found to be as high as 6.77, 7.31, 10.46, and 17.39 with increasing d. The dissipation factor is low over the entire wavelength region, which indicated that the PPNBA thin films have good homogeneity and the higher thickness films are more efficient than those of lower thickness for device applications. The optical conductivity increases with the increase of d, that can be explained the formation of localized states in the gap owing to new defects. Thus, it can be inferred that the PPNBA thin films may find applications in electronic and optoelectronic devices.

Session-IV

Biophysics, Medical & Heath Physics (BMHP)

Invited Talk

IT-IV: The Quantum Design of Photosynthesis

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Three fundamental processes form the basis of natural photosynthesis that efficiently store solar energy in stable products, for later use. The photosynthetic apparatus is constructed of pigments (chlorophylls, bacteriochlorophylls, many different carotenoids) bound to membrane proteins. After the absorption of a solar photon by one of the pigments the electronic excitation is transferred on an ultrafast timescale (10s of femtoseconds to 10s of picoseconds) to a special pigment-protein, the photosynthetic reaction center (RC) where a transmembrane charge separation is driven. Under optimal conditions (low light, water, CO_2) solar photons are captured and transformed into chemical energy with an efficiency (chemical energy out/solar energy in) of about 10-15%. This of course is not the energy yield of a crop! Under not optimal conditions such as high light and stress (draught, low temperature etc) the risk of photodamage increases and the photosynthetic apparatus must be photoprotected. It is obvious that the successful operation of the photosynthetic apparatus depends on a delicate balance between these three fundamental processes. In this talk I will show that one crucial factor is the precise mixing of electronic/excitonic states with charge transfer states often controlled by resonant vibrations. Basically the same physical processes control the speed and balance between ultrafast energy transfer in the light harvesting antenna, ultrafast charge separation and photoprotection: excitons, charge transfer states and resonant vibrations. I will show that quantum coherence between these ultrafast events is the basic physical mechanism. The detailed understanding of these three fundamental processes may be essential for developing and designing artificial biohybrid devices for efficient solar energy conversion and storage.

Work was carried out in collaboration with many guests, postdocs and PhD-students: Eli Romero, Vladimir Novoderezhkin, Natalia Pawlowicz, Fei Ma, Martijn Tros, Md Wahadoszamen, Pavel Maly, Ivo van Stokkum, Joris Snellenburg, Tomas Mancal, Arvi Freiberg, Leonas Valkunas, Bruno Robert etc.

Contributory Talks

BMHP-01: Promising Gradient Waveforms for FRONSAC Encoding for Clinical Brain Imaging.

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Fast Rotary Nonlinear Spatial Acquisition (FRONSAC) is a novel method on accelerated imaging that can significantly accelerate acquisition and consequently reduce the cost of MR imaging. This study reveals the performance of various gradient waveforms for FRONSAC encoding, varying the amplitude, frequency and phase of the oscillation on different channels. Gradient waveforms were tested at a different frequency and two phases (sin and cos). For the high-frequency waveforms, the maximum amplitude is limited by slew limits over one period of the waveform. To test various amplitudes, waveforms were tested at the maximum achievable amplitude for that frequency and half the maximum amplitude. These results demonstrate that FRONSAC encoding does significantly improve undersampling artifacts. These experiments show that dephasing becomes an issue at large moment that are reached when lower frequency waveforms are applied to the strong and steep gradients C3 and S3 gradients. In the case of Z2, the gradient is less strong and steep, so a lower frequency and higher moment are favoured. The results provide an optimized waveform suitable for future studies of clinical sequences and contrasts in human brain imaging.

BMHP-02: Single Molecule Investigation of Tandem G-Quadruplex Structures Formed by Human Telomeric Sequence

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Human telomeric overhangs consist of 100-300 nucleotide long GGGTTA repeats, which can fold into multiple tandem G-quadruplex (GQ) structures. These structures protect and stabilize the telomeres and have been shown to inhibit telomerase activity, which made them an attractive target for anti-cancer drugs. Using single molecule Forster resonance energy transfer (FRET) spectroscopy, we interrogated the accessibility of 24-144 nucleotide long human telomeric DNA molecules (surface-immobilized and donor labeled) with short peptide nucleic acid (PNA) molecules (acceptor labeled) that are complementary to a single GGGTTA repetition. These telomeric overhangs contain 4-24 GGGTTA repeats and can form 1-6 GQ structures when fully folded. However, when not fully folded, certain repeats can be accessed by PNA. PNA strands bind to these open sites on the telomeric DNA for a short period of time prior to dissociation, resulting in discrete FRET bursts as observed in the implementations of the FRETPAINT method. These bursts were analyzed in terms of their dwell times, binding frequencies, and topographic distributions. Both dwell times and binding

frequencies were greater for binding to intermediate regions of telomeric DNA compared to 3 ′ -or 5 ′ -ends. Finally, the binding frequency per telomeric repeat decreased monotonically with increasing telomere length, indicating a length-dependent compaction of the structure. These observations provide a potential framework to understand triggering of senescence or apoptosis when telomeric overhangs become shorter than a critical length (50 nt) where the necessary compaction may not be possible. The higher stability of the ends is consistent with GQ structures protecting telomeres against exonuclease activity.

BMHP-03: DLSCORE: A Deep Learning Model for Predicting Protein-Ligand Binding Affinities

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The cheminformatics community has seen increased success with machine learning-based scoring functions for estimating binding affinities and pose predictions in recent years. Binding affinity prediction plays a vital role in finding novel drugs and is the most time-consuming stage in any drug discovery timeline. Physics-based scoring functions help speed up the process by using computer-aided simulation but such scoring functions are computationally expensive and lack accuracy. Lately, machine learning approaches are proven to boost the performance of traditional scoring functions. In this study, a novel deep learning-based scoring function (DLSCORE) was developed and trained on the refined PDBBind v.2016 dataset using 348 BINding ANAlyzer (BINANA) descriptors. The ensemble of predictors are formed using top-performing neural networks among 55,980 of those and the best set of networks yielded a Pearson R^2 of 0.82, a Spearman Rho R^2 of 0.90, Kendall Tau R^2 of 0.74, an RMSE of 1.15 $kcal/mol$, and an $MAE$of 0.86 $kcal/mol$ for our test set which is comparable to the current state-of-the-art.

BMHP-04: Theoretical Investigation on the Feasibility of Dual Energy X-Ray Imaging of Chronic Obstructive Pulmonary Disease

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Chronic obstructive pulmonary disease (COPD) affects ~200 million people worldwide. Dual-energy (DE) thoracic x-ray imaging reduces anatomical noise and improves visualization of any abnormality in the chest by producing two images acquired at two different energies to reconstruct soft tissue or bone specific image. We propose two-dimensional (2D) unenhanced DE and xenon enhanced (XeDE) x-ray imaging of lung structure and function for the assessment of COPD and theoretically investigate the resulting image quality. We use the human observer detectability index (d') as a figure of merit to detect ventilation defects in XeDE images and emphysema in unenhanced DE images. Our results show that the models of signal, x-ray detector resolution and image noise agree well with previously published data and the disease model also agrees with the established knowledge of detection of emphysema in single energy (SE) radiography. Our results suggest

that DE radiography may improve the detection of emphysema compared to SE x-ray imaging but will unlikely enable detecting mild and moderate stage of COPD. The d' of ventilation defects in XeDE soft tissue suppressed image exceeds the detectability threshold (d'>2) for mild, moderate, and severe COPD at entrance exposure of 18mR. Therefore, XeDE radiography warrants further investigation as a low-dose, low-cost alternative to CT and MRI-based approaches for functional imaging of COPD.

BMHP-05: Pore Size Dependent Molecular Transport to GUVs using COMSOL Simulation

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Biomembranes play a major role in cellular life controlling the transport of different essential substances between the outside and the inside of cells. As a mimic of biomembranes of cells, lipid membranes of giant unilamellar vesicles (GUVs) with diameters 10 μm or more were used to investigate the pore formation induced by various membrane-active agents such as antimicrobial peptides [1]. Pore formation and molecular transport/leakage rate is important to investigate the kinetics molecular transport through nanopores in the membranes of GUVs. Recently, simulation work has been performed to explore molecular transport into vesicles through a single nanopore from the outside to the inside of vesicles using COMSOL simulation [2, 3].

The sizes of GUVs and fluorescent probes were considered based on experimental data [4]. In this study, investigate the molecular transport/leakage rate into the GUVs through nanopore with respect to pore size to unveil the kinetics molecular transport through nanopores in the membranes of GUVs. We have considered here for different fluorescent probes (AFSBTI, FITC-BSA, TRD-3k, TRD-10k and TRD-40k) and for various sizes of pore size. The obtained molecular transport/leakage rate increased with increase of pore size (Fig) that indicates good correlation of our simulation results with experimental findings [4]. The measured values of rate constant obtained from this simulation are very similar to the reported experimental data.

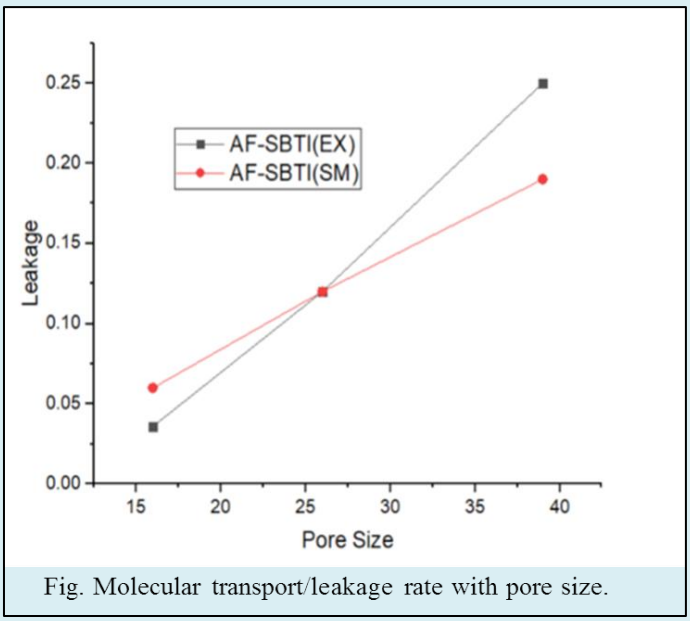

Fig. Molecular transport/leakage rate with pore size.

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BMHP-06: Continuous Radiation Monitoring at Atomic Energy Centre Dhaka Campus using Thermoluminescent Dosimeters

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Ionizing radiation has many beneficial applications at radiological facility like Atomic Energy Centre Dhaka (AECD) for routine service, training, research & development activities. Radiation generating equipments and radioactive materials in a radiological facility is to be handled very carefully for the protection of the people and the environment from undue radiation hazard. The objective of the study is to continuous indoor radiation monitoring at AECD campus and evaluation of radiation risk on workers & public. Continuous radiation monitoring was carried out at the AECD campus from August-October 2020 using the Thermoluminescent Dosimeters. Twenty locations were selected at the AECD campus for continuous radiation monitoring and each location one Thermoluminescent Dosimeter was placed at one meter above the ground. The annual effective dose to workers and public were calculated based on the continuous radiation monitoring data and ranged from 0.606 ± 0.031 mSv to 0.801 ± 0.0.042 mSv with an average of 0.707 ± 0.053 mSv. The excess life-time cancer risk (ELCR) on workers & public were evaluated based on the annual effective dose and ranged from 2.486 X 10^{-3} to 3.287 X 10^{-3} with an average of 2.900 X 10^{-3}.The average annual effective dose and ELCR on workers & public were lower than those of the worldwide permissible values. Continuous radiation monitoring at the radiological facility is very important for detection of the radiation generating equipments malfunctions and improper handling of the radioactive materials. The study would help for reduction of radiation risk on workers & public at radiological facility and for detection of abnormal situation arising from the radiation hazard.

BMHP-07: Real-time Indoor Radiation Monitoring at INMAS Mitford Hospital Campus following In-Situ Method and Estimation of Radiological Risk on Worker & Public

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The usage of radiation generating equipments and the radioisotopes in nuclear medicine for diagnostic & therapeutic procedures to patients are increasing worldwide. Radiation worker in nuclear medicine department is more vulnerable than other departments in the hospital, because worker of the nuclear medicine department used to handle unsealed radioactive materials. If indoor workplaces in the hospital contain radiation while handling unsealed radioactive materials due to spill, there is a probability for getting higher radiation dose to worker and public. Therefore, real-time indoor radiation dose rate monitoring is very important for detection of radiation hazard in the hospital. The study was conducted at Institute of Nuclear Medicine and Allied Sciences (INMAS), Mitford Hospital campus from February-March 2020 using digital portable radiation monitoring devices along with GARMIN eTrex GPS device for marking out each monitoring point (MP). 24

MPs were selected at indoor places of INMAS Mitford Hospital campus for collection of the real-time dose rate following In-Situ method. The measured dose rates were found to be in the range of 0.01 - 10.12 $\mu Sv.h^{-1}$ with an average of 1.459 ± 1.767 $\mu Sv.h^{-1}$. The annual effective dose to the worker & public due to indoor radiation was ranged from 0.016-16.451mSv and the mean was found to be 2.371 ± 2.874 mSv. The highest annual effective dose (5.952 mSv) was found at patient's waiting room after injecting radioisotopes. The excess life-time cancer risk (ELCR) on worker were ranged from 6.676 X 10^{-5}-6.756 X 10^{-2}. Public should not enter into the injected patient's waiting room unnecessarily.

BMHP-08: Spatial Distribution and Contamination of Trace Elements in Surface Sediments of the Kaptai Lake, Bangladesh Using Neutron Activation Analysis

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In this study, total concentrations of 25 major, minor, and trace elements (Na, Al, K, Sc, Ti, V, Cr, Mn, Fe, Co, Zn, As, Cs, La, Ce, Sm, Eu, Tb, Dy, Yb, Lu, Hf, Ta, Th, and U) in surface sediments of the Kaptai lake, Bangladesh were determined by using research reactor-based neutron activation analysis (NAA) technique. To identify concentration variations and pathways of elements, sediment samples were collected from 32 different locations of the lake. Samples were neutron- irradiated using a pneumatic transfer system of the 3 MW TRIGA research reactor at Bangladesh Atomic Energy Commission, and gamma-ray activities of the product radionuclides were measured using a high-resolution HPGe detector system. For the quality control analysis of the relative standardization approach of NAA, reference materials (RMs): IAEA-Soil-7, IAEA-SL-1 (lake sediment), and NIST-1633b were used in this study. When compared with upper continental crustal (UCC) average values, it is observed that the mean concentration of Ti, Zn, As, Cs, La, Ce, Sm, Eu, Dy, Yb, Lu, Hf, Ta, Th, and U show elevated values with respect to UCC. Assessment of elemental contamination, using different pollution indicators, suggests that sediments of the Kaptai lake are minorly enriched by Zn, As, Cs, REEs, Hf, Ta, Th, and U. The calculated pollution load index (PLI) values also suggest deterioration of sediment quality in 3 sampling stations. Pearson's correlation matrix of the elements was calculated to establish relationships among elements and their origins which indicates that Fe, Co, As, and Cs are of similar origins. These results are necessary for future monitoring related to elemental contamination of the lake ecosystem.

Session-V

Theoretical Condensed Matter Physics (TCMP)-I

Invited Talk

IT-V: Tuning Properties of Two-Dimensional Materials for a Sustainable Future

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In the pursuit of a sustainable future, the last decade has seen a concerted effort in accelerating the discovery of materials for energy needs, thanks to a large extent to the Materials Genome Initiative (MGI). After some reflections on how this initiative has led to a research paradigm shift, naturally embracing the intertwining of theoretical and experimental research, and now data analytics, I will focus on a few materials which have captured the imagination of scientists worldwide. As with graphene, which consists of a single sheet of carbon atoms exfoliated from graphite, another common lubricant, molybdenum disulphide (MoS_2), has shown remarkable optical properties when peeled off as single sheet consisting of a layer of molybdenum atoms sandwiched between two layers of sulfur atoms. With an eye on optoelectronic applications that could rival silicon, a host of single-layer, bilayer, and hetero-structures of transition metal dichalcogenides, and other van der Waals materials have been investigated. Perhaps even more appealing is a layer of boron and nitrogen atoms on a hexagonal lattice (*h*-BN), emanating from another rugged old material, that could serve as a single photon emitter (for possible applications in quantum computing) or as a catalyst for sequestration and conversion of carbon dioxide to value added products such as methanol and formic acid, with efficacy comparable to that of the expensive transition metal, platinum. I will present some results from our work that provides a framework for manipulating the functionality of these interesting two-dimensional materials for industrial applications.

Contributory Talks

TCMP-01: Multiple Superexchange Interactions for Ferromagnetic Insulator in Rare Earth oxides

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Insulating ferromagnets are deficient, especially at room temperature and the origin of their localized parallel spin exchange interaction particularly for f electron systems is ambiguous and yet to be understood properly. In rare earth oxides, cations carry magnetic moment with their f-electrons which has highly localized character and can be promising for ferromagnetic insulating nature. We explored CeO_2 associated with oxygen vacancy and evaluated the doping effect and found that oxygen deficient Pr doped CeO_2 exhibits ferromagnetic nature while doped Pr and some Ce carries magnetic moments upon reducing to +3 ionized state from their pristine +4 states. These reduced Pr and Ce assemble the superexchange pair with intervening oxygen ion and their small degree of orbital splitting lifted due to non-uniform potential on SEI pair and allow them to occupy multiple 4f orbitals which eventually outnumber the ferromagnetic superexchange interactions over antiferromagnetic one in the virtue of multiple superexchange interaction to promote magnetic ground state. On the contrary, while only Pr or Ce construct the superexchange pair, due to the uniform potential environment on SEI pair, the degree of orbital splitting sustained, and ferromagnetic ordering suppresses by equal number of antiferromagnetic interactions. The concept of multiple superexchange interactions was elaborated based on Goodenough-Kanamori-Anderson rules for all 7 4f orbitals symmetry and making use of first principal calculations a prediction of occupied orbitals related magnetic interaction is presented.

TCMP-02: The Adsorption of Oxygen on Bimetallic Pd_3M_2 Clusters (M = Ag, Au, Co, Cu, Mn, Ni, Pt and Ru) with and without Alumina Support by Density Functional Theory

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We use density functional theory to systematically investigate the adsorption of oxygen on the bimetallic Pd_3M_2 clusters (M = Ag, Au, Co, Cu, Mn, Ni, Pt, and Ru) with and without supported alumina. This is because small bimetallic clusters with high surface area to volume ratio often offers, higher stability, greater selectivity, and sometimes superior activity than the pure metal counterparts. We explore different adsorption sites for molecular oxygen, which can be oriented in a vertical or horizontal direction with respect to the cluster, as well as atomic oxygen on these bimetallic Pd_3M_2 clusters. We investigate how the presence of an alumina support affect the molecular and atomic oxygen adsorption energy on these bimetallic clusters. Moreover, we will present the effect of oxygen adsorption on the electronic properties of these Pd_3M_2 clusters

with and without alumina support. Bader charge analysis is performed to probe how the charges are transferred between the atomic and molecule oxygen with these bimetallic clusters and its effect is compared with the presence and absence of the alumina substrate.

TCMP-03: A First-principles Investigation of Physical Properties of Topological Weyl Semimetals Ta*X* (*X* = P, As)

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In recent times, topological Weyl semimetals have attracted enormous interest of the scientific community both from the points of view of fundamental physics and possible applications. In this study, the structural, elastic, mechanical, electronic, bonding, acoustic, thermal and optical properties of Ta*X* (*X* = P, As) Weyl semimetals have been carried out in detail via first-principles method using the density functional theory. The elastic constants and moduli shows that both the compounds possess low to medium level of elastic anisotropy, reasonably good machinability, mixed bonding characteristics with ionic and covalent contributions, brittle nature and relatively high Vickers hardness with a low Debye temperature and melting temperature. The electronic band structure calculations reveal clear semi-metallic features with quasi-linear energy dispersions in certain parts of the Brillouin zone near the Fermi level. The reflectivity spectra exhibit almost non-selective behavior over a wide range of photon energy encompassing visible to mid-ultraviolet regions. Ta*X* (*X* = P, As) compounds are predicted to be efficient absorber of ultraviolet radiation. The refractive indices are high in the infrared to visible range. The energy dependent optical parameters show close agreement with the underlying electronic band structure and electronic density of states features.

TCMP-04: DFT+U Study of the Structural, Magnetic and Optical Properties of Pure and (Fe, Co) Co-doped CuO Nanoparticles

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The semiconducting material Copper oxide (CuO) has very interesting structural and optical properties. Transition metal doped and co-doped CuO nanostructures have great potential to use in memory device and many optoelectronic applications. The structural, electronic, optical and elastic properties of pure and (Fe, Co) co-doped CuO (Cu1-x-yFexCoyO) is studied by using Density Functional Theory (DFT). To take the onsite Coulomb repulsion into account for this strongly correlated material the DFT+U approach is used. The structural relaxation is done for different doping position and spin configuration and found that the most favorable structure have C2/c symmetry with antiferromagnetic spin configuration. The electronic bandgap is reduced by an amount of 0.8211 eV after the (Fe & Co) co-doping which in turn make the nanoparticles more suitable for p-type applications. The non-magnetic CuO become magnetic after the doping of Fe and Co atom. This improvement of ferromagnetic properties is in good agreement with the experimental findings available

in the literature. The density of states, band structure and dielectric properties are also studied. Our findings confirm the previously obtained experimental optical properties and reveals the exciting properties of (Fe & Co) co-doped CuO that are yet to be discovered through the experimental efforts.

TCMP-05: Calculation of Electrical Resistivity for Liquid Binary Cu_xAg_{1-x} Alloys

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Electrical resistivity of liquid binary Cu_xAg_{1-x} alloys is calculated using the extended Ziman's formula developed by Faber and Ziman at 1423 K. Form factor, $V_{ij}(q)$, and partial structure factor, $S_{ij}(q)$, are the key ingredients of this calculation. For $V_{ij}(q)$, we have chosen Bretonnet-Silbert (BS) pseudo-potential with Ichimaru-Utsumi (IU), and Vashishta-Singwi (VS) local field correction functions. For $S_{ij}(q)$, we have chosen linearized Weeks-Chandler-Andersen (LWCA) thermodynamic perturbation theory. Calculated results of electrical resistivity comparing with the available experimental data suggest that the choice of VS local field correction function in the potential is important than IU local field correction function. It is also observed that the applied theory with both local field correction functions works well for Ag-rich alloys than those of Cu-rich alloys. To explain the resistivity of Cu-rich alloys more accurately a further study with more sophisticated theory is required.

TCMP-06: Density Functional Study of Pressure Dependent Physical Properties of SnS and Sb_2S_3

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The pressure dependent physical properties of tin sulphide (SnS) and antimony sulphide (Sb_2S_3) have been investigated by first principles density functional theory (DFT) based calculations. The structural, elastic, bonding, optoelectronic and some thermophysical properties of both these compounds have been explored in details. For tin sulphide, results show that it undergoes semiconductor (with a band gap of 0.592 eV) to semimetal transition as the pressure increases. On the other hand, antimony sulphide, which is a semiconductor with a band gap of 1.153 eV at ambient, undergoes semiconductor to semimetal transition at a pressure about 20 GPa. The elastic properties including the anisotropy indices of SnS and Sb_2S_3 have been investigated. The pressure dependent Debye temperatures have been calculated. Energy dependent optical constants show clear correspondence with the calculated electronic band structure and density of states features. Both SnS and Sb_2S_3 possess attractive optical absorption and reflectivity spectra which might be useful for optoelectronic device applications.

TCMP-07: A DFT with Advanced Functionals (DFT+U) Study of Cubic and Hexagonal ZnX (X= O, S, Se, Te) for Potential Optoelectronic Device Application

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Transition metal chalcogenides (TMCs) compounds are technologically important, specifically for solar cells and other optoelectronic devices. The computational simulation on structure and optoelectronic properties has been done using renown ab initio density functional theory (DFT) within GGA, and GGA+U for similarities-dissimilarities of ZnX (X = O, S, Se, and Te) from the view of underlying fundamental physical mechanism. The General Gradient Approximation (GGA) overestimate the band gap and misplaces the valence band which makes the DFT study far away from the experimental findings. This errors in band gaps and related parameters originate from strong Coulomb correlations, which are found to be highly significant in ZnO. To compensate this theoretical and experimental miscalculations, the study is continued by using the Hubbard-U scheme incorporated with both Zn 3d states and their respected valence p state with Coulomb or electric potential energy (U) correction, range 0–20 eV for hexagonal ZnO, and 0-10 eV for other 3 compounds. These compounds are found to be direct band gap semiconductors which might be usable as replace of silicon. Thorough study of reflectivity, absorption, refractive index, and conductivity have been studied in the visible, and UV region for the suitability of optoelectronic application. This review also provides graphical, and tabulated values extracted from earlier works on optoelectrical properties.

Session-VI

Experimental Condensed Matter Physics (ECMP)

Invited Talk

IT-VI: Band Structure Engineering and Heterojunction of Two-dimensional Transition Metal Dichalcogenides

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The ability to modify the electronic structure of a semiconducting material via doping or defect engineering is of significant importance for the development of many novel applications in emerging nano-electronics, optoelectronics, sensing, catalysis, and energy devices. In this talk, I will discuss my group's recent effort in tailoring the electrical properties of semiconducting transition metal dichalcogenide (TMD) materials via (i) defect engineering using mild oxygen plasma, and (ii) interfacial charge transfer via deposition of small molecules or metallic nanostructures. In particular, I will show that the mobility, on-current, and resistance of monolayer and few layer MoS_2 samples vary exponentially when exposed to mild oxygen plasma. Photoluminescence, Raman, and X-ray photoelectron spectroscopy were used to elucidate the physical mechanism responsible for the band structure modification which resulted in tunable electrical properties. Lateral heterojunction was fabricated with selective patterning that show gate tunable current rectification behavior. I will also discuss how nanostructures of Au deposited on MoS_2 can tune the potential landscape of MoS_2 as revealed from room temperature and low temperature electronic transport measurements. Finally, I will discuss chemical doping of large area MoS_2, $MoSe_2$ and $PdSe_2$ thin films by benzyl viologen molecule and show how this technique can be used for scalable fabrication of lateral heterojunctions.

Contributory Talks

ECMP-01: Improved Electrical Properties of *in-situ* SiNx Passivated AlGaN/GaN HEMT by Tailoring the Stoichiometry of the Passivated Layer

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Due to intrinsic wide bandwidth and high breakdown voltage, polar semiconductor gallium nitride (GaN) based high electron mobility transistors (HEMTs) is the primary choice for next generation high-frequency power amplification from the S-band to W-band with high power-added efficiencies (PAE) and thermal stability. We report *in-situ* SiNx passivation of AlGaN/GaN HEMTs grown by MOCVD without surface damage at typical HEMT growth conditions. Higher SiNx growth rate, when produced by higher SiH4 reactant gas flow, enables faster lateral coverage and quicker coalescence of the initial SiNx islands thereby suppressing SiH4 induced III-Nitride etching. The effect of *in-situ* SiNx passivation on the structural properties of AlGaN/GaN HEMTs has been evaluated using high resolution x-ray diffraction. Electrical properties of the passivated HEMTs were evaluated by measuring clover-leaf Van der Pauw Hall structures. The key findings include, (a) a correlation of constituent gas chemistry with SiNx stoichiometry, (b) the degree of suppression of strain relaxation in the barrier layer can be optimized tailoring the SiNx stoichiometry, (c) Optimum strain relaxation by tailoring the stoichiometry of the passivating SiNx layer can result near perfect AlGaN/AlN/GaN interface for the quantum well, thereby reduces the carrier scatterings and improves mobility. With optimized conditions, low sheet resistance and high electron mobility are obtained. At 10 K, a sheet resistance of 33 Ω/sq and 16500 cm2/V-s mobility is achieved while at 300 K, the sheet resistance is 336 Ω/sq with a mobility of 2020 cm2/V-s and a sheet charge density of 0.78×1013 cm-2.

ECMP-02: Drastic Enhancement of Efficiency in DSSC by Electrosorption

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Herein, we report dye-sensitized solar cells (DSSCs) made of dye stained TiO_2 semiconductor photoanode fabricated using a quick and novel electrosorption assisted dye-staining process. Electrosorption, through the application of electrochemical potential, can manipulate the interaction of target compounds (in this case "dye") with an electrode surface. To demonstrate the importance of the electrosorption assisted dye-staining process, two commercially available metal-based dyes (N719 and Z907) and two metal-free dyes (D2d = (Z)-2-cyano-3-(4-((E)-2-(6-(4-methoxyphenyl)-9-octyl-9H-carbazol-3-yl) vinyl) phenyl) acrylic acid and T-SB-C = (E)-2-cyano-3-(4-((E)-4-(diphenylamino) styryl) phenyl) acrylic acid) having carboxylic acid type anchoring group were chosen. By this process, the dye loading realized on the photoanodes was more than that of the

conventional soaking process. In case of N719 dye, dye loading was enhanced about 100 % from 0.58 $x10^{-7}$ to 1.21 $x10^{-7}$ mol cm^{-2}, and power conversion efficiency (PCE) by 35 %. The electrosorption assisted dye-staining process discussed in this study requires only an hour to fabricate photoanode versus 12 to 48 h required for the conventional soaking process.

ECMP-03: Electron Transport in Photochromic Rare-earth Metal Oxy-hydride Thin Films

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Photochromic materials reversibly turn opaque from a transparent state upon exposure to radiation of optical wavelength. In photochromic rare-earth metal oxy hydride (REMHO) thin films, this effect is color-neutral which has established them as a possible future candidate of smart glasses [1]. This photochromic effect is associated with an instant switching in resistivity as well (sharp decrease from 1012Ω to 108Ω). Combination of these two phenomena can be applied in developing optical sensors. But to what extent are these two phenomena related? To answer this, we grew thin films of yttrium hydride on glass substrates by reactive magnetron sputtering which upon exposure to air form yttrium oxy hydride. The thickness of the films and the depth profile of its constituents were extracted from Ion Beam Analysis methods. We observed the kinetics of the photochromism by recording the time-resolved transmittance of the films during photodarkening and bleaching using a UV-vis spectrometer. The electric transport property of the films was characterized simultaneously by measuring the resistivity of the films. We observed that photoconductivity is a bulk effect that saturates above 500 nm thickness. Illumination from the substrate side showed a larger decrease in resistance during photodarkening but slower relaxation during bleaching compared to illumination from the film side. The relaxation curve from the resistivity measurement did not show any specific trend unlike the optical relaxation which was always exponential. Moreover, we observed photoconductivity irrespective of photochromism. We also quantified the wavelength and intensity dependence of the photoconductive response of REMHO thin films.

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ECMP-04: Studies on Dielectric and Photocatalytic Properties of Zeolite/MWCNT Nanocomposite

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The composites of OH functionalised Multiwalled Carbon Nano Tubes (MWCNT) and the different zeolite qualities (Zeolite/MWCNT-1 and Zeolite/MWCNT-2) have been prepared. The structural characterisation for all samples was done using the XRD technique. It turns out that the XRD peak strength of the composites is decreasing, confirming the formation of composites. Further studies have also been conducted to study dielectric studies and photodegradation of composites. It is noted that electric properties such as AC conductivity, dielectric constant, and loss tangent of Zeolite/MWCNT-1 were improved significantly as compared to Zeolite/MWCNT-2. This shows that the example is the proficient manufacture of capacitors. Zeolite/MWCNT-2 is utilized as a photocatalyst for degradation of methylene blue (MB) colour arrangement under light illumination. It displays high catalytic action within the sight of apparent light. Henceforth Zeolite/MWCNT-2 composites might be utilized to adjust the degradation property and may broaden likely applications for degradation of organic pollutants.

ECMP-05: Synthesis and Characterization of GO Based PVA Nanocomposites Based on GO using Reduced Percentage of GO Nanofillers

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Graphene-based polymer composites are gaining interest as they hold promising angles on diverse applications. Here, Graphene Oxide (GO) based Polyvinyl Alcohol (PVA) nanocomposites (PVA-GO) have been prepared by employing a facile solution casting method. Low concentrations of GO nanofiller (0.25%, 0.50%, 0.75%, and 1.0%) were used and their result over the distinct substantial characteristics of the nanocomposites was evaluated. The different features of the as-synthesized nanocomposites such as optical, structural, chemical, and thermal properties were identified by UV-Vis spectroscopy, X-ray diffraction (XRD), Fourier transform infrared spectra (FTIR), and Thermo-gravimetric analysis (TGA), respectively. From the structural analysis of the nanocomposite, it is evident that a reduction in crystallinity caused by the amalgamation of the GO nanofiller. FTIR study shows improved interaction between the GO nanofiller and PVA matrix. The incorporation of GO was found to reduce the optical band gap of the nanocomposite both for the direct and indirect transition. The Urbach energy of the nanocomposite increases with the increase of the GO concentration suggests the formation of localized states causing a reduction in the optical band gap. PVA-GO nanocomposites with improved and tunable physical properties synthesized from a simple and economic route may pave a new horizon for polymer-based optoelectronic devices.

ECMP-06: Thickness Dependent Optical Properties of the AC Plasma Polymerized 3,4-Ethylenedioxythiophene Thin Films

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Plasma polymerization is a distinctive technique for direct polymeric thin films deposition from different organic monomers. The organic compound 3,4-ethylenedioxythiophene (EDOT) has been chosen as monomer to deposit plasma polymerized EDOT (PPEDOT) thin films. The polymerization is carried out by using a capacitively coupled glow discharge reactor by optimizing the plasma parameters, where the plasma is created at line frequency (50 Hz). Thicknesses of the thin films are varied by synthesizing PPEDOT thin films for different deposition times and powers, where the thicknesses are measured by Multiple-Beam interferometer technique. Different optical parameters such as the absorbance, absorption coefficient, direct and indirect band gap energies, Urbach energy, extinction coefficient, refractive index, optical conductivity, skin depth are obtained from UV-visible spectra of the deposited PPEDOT thin films and are correlated to understand the applicability of the PPEDOT thin films. From the UV-Vis analysis, it is observed that the values of direct band gap energy, $E_{g(d)}$, varies from 3.94 to 3.86 eV and that of the indirect band gap energy, $E_{g(i)}$, varies from 3.62 to 3.20 eV for the PPEDOT thin films of different thicknesses. The decrease of $E_{g(d)}$ and $E_{g(i)}$ values with the increasing thicknesses is due to the increase in fragmentation/cross-linking in the bulk of the material due to the impact of plasma on the surface of the thin films with plasma duration. The values of the Urbach energy, E_u varies from 0.00364 to 0.00258 eV with the variation of thickness due to the increase of disorder in the PPEDOT thin films.

ECMP-07: Wide Bandgap Ga_2O_3 Based Alloy by Pulsed Laser Deposition

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Thin film ultrawide bandgap Ga_2O_3 based alloys are promising in high power electronic, deep UV photonic devices, gas sensors, magnetic and nuclear detectors applications. These alloys can be epitaxially deposited by pulsed laser deposition on (0001) plane Al_2O_3 substrates and open the possibility of the development of heterostructure devices that involves HEMT and quantum well structures with a variety of functionalities. Alloy containing Fe can be used for wide bandgap spintronic and optoelectronic applications. This report will present the epitaxial growth of $Ga_{1-x}Fe_x)_2O_3$ thin films as a function of x using pulsed laser deposition, as well as a discussion of the impact of growth parameters on the crystal structure, surface properties and optical bandgap tuning.

ECMP-08: MBE Growth of High-Quality GaAs on C-plane Sapphire Substrate

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Heteroepitaxy of III-V semiconductor is a well-established field. Generally, the term heteroepitaxy is used to denote the growth of dissimilar materials having similar crystal structure but different lattice constant. Very few examples exist in literature regarding single-crystal epitaxy of two semiconductors with dissimilar crystal structures such as cubic on wurtzite or cubic on trigonal. There have been a few works regarding cubic SiGe growth on a trigonal sapphire substrate. In this report, we discuss the growth of quality GaAs buffer on c-plane sapphire. Our motivation to grow GaAs on sapphire is based on its potential use in III-V microwave photonics, optoelectronics and electronics owing to the properties, such as, a large contrast in refractive index between GaAs and sapphire, the high resistivity of sapphire substrate and the transparency of the sapphire substrate near the III-As band gap.

When grown on c-plane sapphire, GaAs tend to grow along the [111] orientation. In our experiments we have observed that the growth of GaAs on sapphire has a small range of parameter for best quality material. In this window, our samples show a surface RMS roughness as low as 1.6 nm; a rocking curve linewidth comparable to the GaAs substrate at 90 arcsec, good photoluminescence efficiency, and suppression of twinning in GaAs to less 0.1%. The latter was accomplished by utilizing different growth strategies, such as, a low temperature initial layer, multiple annealing cycles and by optimizing growth parameters (growth temperature and arsenic flux).

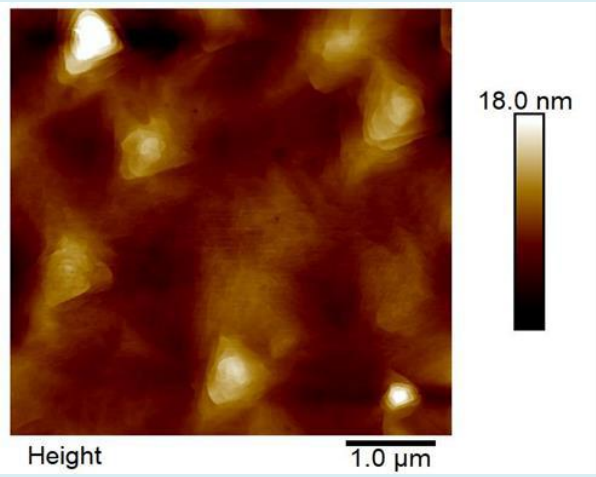

Figure 1: AFM image of GaAs/Sapphire.

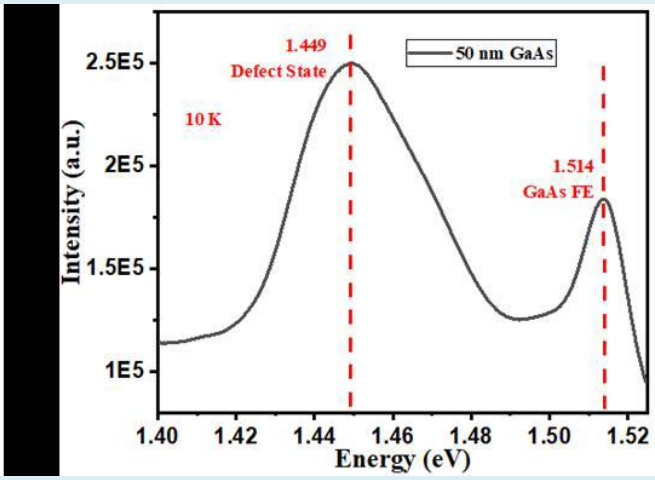

Figure 2: PL from GaAs buffer. GaAs FE denotes the free exciton peak.

Session VII

Theoretical Condensed Matter Physics (TCMP)-II

Invited Talk

IT-VII: Bosons in High-T_c Cuprates: Where Do We Stand?

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Identification of the bosonic degrees of freedom mediating Cooper pairing in hole doped copper oxide superconductors remains a contentious issue after nearly thirty-five years of the discovery of these high-T_c compounds. We present a critical evaluation of the present understanding of the *d*-wave pairing of charge carriers in these strongly correlated electronic systems with varying hole concentration. Possible roles of charge density waves (CDW) and spin density waves (SDW) are examined. Possibility of conventional phonon mediated superconductivity has also been explored. The changes in the charge and spin excitation spectra due to the variation of the doped holes within the CuO_2 planes of cuprates often yield contradictory results as far as the formation of phase coherent Cooper pairs are concerned. The doping dependent isotope exponent is highly unconventional. All these indicate that a single dominant bosonic mode of definite origin might be inadequate to reproduce the complex electronic phase diagram of hole doped cuprates in the superconducting state.

Contributory Talks

TCMP-08: Effect of Dilute Magnetism in a Topological Insulator

Firoza Kabir[1], M. Mofazzel Hosen[1], Xiaxin Ding[2], Christopher Lane [3,4], Gyanendra Dhakal[1], Yangyang Liu[1], Klauss Dimitri[1], Christopher Sims[1], Sabin Regmi[1], Anup Pradhan Sakhya[1], Luis Persaud[1], John E Beetar[1], Yong Liu[5,6], Michael Chini[1], Arjun K. Pathak[7], Jian-Xin Zhu[3,4], Krzysztof Gofryk[2], and Madhab Neupane[1,*]

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Three-dimensional topological insulator (TI) has emerged as a unique state of quantum matter and generated enormous interests in condensed matter physics. The surfaces of a three-dimensional (3D) TI consist of a massless Dirac cone, which is characterized by the Z_2 topological invariant. Introduction of magnetism on the surface of a TI is essential to realize the quantum anomalous Hall effect and other novel magneto-electric phenomena. Here, by using a combination of first-principles calculations, magneto-transport, and angle-resolved photoemission spectroscopy (ARPES), we study the electronic properties of gadolinium (Gd)-doped Sb_2Te_3. Our study shows that Gd doped Sb_2Te_3 is a spin-orbit-induced bulk band-gap material, whose surface is characterized by a single topological surface state. We further demonstrate that introducing diluted 4*f*-electron magnetism into the Sb_2Te_3 topological insulator system by the Gd doping creates surface magnetism in this system. Our results provide a new platform to investigate the interactions between dilute magnetism and topology in magnetic doped topological materials.

TCMP-09: Fermi Surface Mapping of Non-Trivial Topological Semimetal Candidate $CaSn_3$

K A M Hasan Siddiquee[1,*], Riffat Munir[1], Charuni Dissanayake[1], Xinzhe Hu[2], Swapnil Yadav[2], Yasumasa Takano[2], Eun Sang Choi[3], Talat S Rahman[1], Duy Le[1], Yasuyuki Nakajima[1]

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Theoretically predicted, binary stannide $CaSn_3$ is one of the promising candidates of topological semimetals (TSMs) [1]. It undergoes superconductivity at $T_c \approx$ 4.2K [2], which provides an excellent platform for understanding the interplay between topological physics and superconductivity. To understand this interplay, knowing the fermiology of the normal state is necessary. Here, we present a de Haas–van Alphen (dHvA)

oscillations study for $CaSn_3$ single crystals via torque magnetometry in high magnetic fields up to 35T. Together with the density functional theory calculations, we will map the Fermi surfaces of non-trivial topological semimetal candidate $CaSn_3$.

[1] S. Gupta, R. Juneja, R. Shinde, and A. K. Singh, Journal of Applied Physics **121**, 214901 (2017).
[2] X. Luo, D. F. Shao, Q. L. Pei, J. Y. Song, L. Hu, Y. Y. Han, X. B. Zhu, W. H. Song, W. J. Lu, and Y. P. Sun, J. Mater. Chem. C **3**, 11432 (2015).

TCMP-10: Search for a Light Pseudoscalar Higgs Boson in the Two Higgs Doublet Model using Data from the Large Hadron Collider (LHC)

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A search is presented for a light pseudoscalar Higgs boson (a) using data collected by the CMS experiment at LHC, at centre-of-mass of energy of 13 TeV. The study looks into the decay Higgs boson (H) via the $H \rightarrow aa \rightarrow \mu\mu\tau\tau$ channel. The Higgs boson can be both standard-model-like (125 GeV) or heavier. The pseudoscalar mass falls within the range $m_a \epsilon [2m_\tau, m_H/2]$. The large mass difference between the Higgs and the pseudoscalar means that the final tau lepton decay products are highly boosted in the decay direction and collimated. A modified version of tau reconstruction is used to account for the highly overlapping decay products. The modified reconstruction technique gives higher reconstruction efficiency over the standard tau reconstruction and hence better signal significance and background rejection. This technique also becomes useful when looking into various final states, especially the ones where one of the taus decays hadronically while the other decays leptonically (μ/e). The performance of the altered reconstruction technique, as opposed to the standard tau reconstruction, is also presented. The results from the 2016 and 2017 CMS datasets will be shown, corresponding to integrated luminosities of 35.9 fb^{-1} and 41.5 fb^{-1} respectively.

TCMP-11: Justification of the Scaling Law of Dzugutov for Diffusion Coefficients of Liquid $Cu_xAg_{(1-x)}$ Alloys

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The scaling law of Dzugutov for the diffusion coefficient of liquid transition binary alloys (Cu_xAg_{1-x}) has been justified. Structure dependent reduced diffusion coefficient and thermodynamic excess entropy are required for justification. To calculate them, we have determined effective Hard Sphere (HS) diameter (σ) and excess

entropy (S_{ex}) using pair correlation function, $g$ij(r). For $g$ij(r), we have used linearized Weeks-Chandler-Andersen (LWCA) thermodynamic perturbation theory along with Bretonnet-Silbert (BS) pseudo-potential model with Ichimaru-Utsumi (IU), and Vashishta-Singwi (VS) local field correction functions. σ is estimated from the intersection of the transcendental equation of LWCA and S_{ex} is calculated using two two-body (S_2) and many-body approximation (S_E) of Carnahan and Starling. Comparing with experimental and simulated data, S_E results are found to be closer than that of S_2. IU local field correction function provides reliable values for diffusion coefficients than those obtained using VS local field correction function except for Cu-rich alloys which are deviated much from experimental and simulated data. The justification behind this inconsistency requires a further study with a more sophisticated theory.

TCMP-12: Experimental and First Principles Look into $BiVO_4$

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Bismuth vanadate ($BiVO_4$, BVO) is perhaps the most studied photoanode material for photo- electrochemical (PEC) generation of clean solar fuels such as hydrogen. Out of its three different polymorphs; namely pucherite, dreyerite and clinobisvanite, the last one having a monoclinic scheelite (ms) structure is shown to have superior PEC performance. Here we attempt to synthesize phase pure ms-BVO using a facile solid state reaction technique aided with a two-step sintering process (400-500^o C). The ms phase of the synthesized BVO samples has been confirmed from Rietveld analysis of the powder X-ray diffraction pattern and room temperature Raman spectroscopy. The optical band gap measured in the range of 2.38 - 2.58 eV from the UV-VIS-NIR diffuse reflection spectroscopy further corroborates the ms-BVO structure. Moreover, we present first principles simulations for crystallographic parameters, phononic and electronic density of states and energy band structure of ms-BVO within the framework of Density Functional Theory to support afore mentioned experimental observations. The ms-BVO photoanode with variable structural and optical properties could be a promising candidate for PEC generation of solar fuels.

TCMP-13: A Theoretical Based Study on Atomic Transport Properties of Liquid Simple Metals

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Self-diffusion coefficient, *D*, of some liquid simple metals namely Bi, Tl, Sn, Cd, Pb, In, Sb and Zn has been investigated using linear trajectory and small step diffusion theories. Friction coefficients originated from the hard, soft and crossed hard-soft parts of the potential are the main ingredients of the applied theories. We have chosen potential derived from Brettonet–Silbert (BS) pseudopotential model. For structure dependent calculation, Variational modified hypernetted chain (VMHNC) integral equation theory has been applied. From the comparison with available experimental data and other theoretical values, we observe that the calculated values using linear trajectory theory are more reliable than those obtained using small step diffusion theory for the concerned systems. The probable reason behind may be the contribution coming from the crossed hard-soft forces which is neglected in the small step diffusion theory.

TCMP-14: Physical Properties of Transition Metal Dichalcogenides ZrX_2 (X = S, Se, Te): First-principles Insights

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Transition metal dichalcogenides (TMDCs) are important compounds from the view of technological applications. In this study, structural, elastic, bonding, optoelectronic, vibrational and some thermo-physical properties of three binary TMDCs are investigated via density functional theory (DFT). Elastic anisotropy indices, atomic bonding character, optoelectronic properties, thermo-physical features including melting temperature, minimum phonon thermal conductivity and vibrational properties including phonon dispersion and phonon DOS are studied for the first time. The electronic band structures show that ZrS_2 and $ZrSe_2$ are semiconductors with direct and indirect band gaps, respectively, while $ZrTe_2$ is a conductor. All the TMDCs under investigation possess significant elastic/mechanical anisotropy. ZrX_2 (X = S, Se, Te) compounds are fairly machinable, and ZrS_2 and $ZrSe_2$ are reasonably hard. $ZrTe_2$, on the other hand, is markedly softer. Both covalent and ionic bondings contribute in the crystals. Optical absorption coefficients show that ZrX_2 (X = S, Se, Te) are efficient absorber of ultraviolet radiation. The reflectivity spectrum, $R(\omega)$, stays over 50% in the energy range from 0 eV to ~20 eV for $ZrTe_2$. Therefore, $ZrTe_2$ has wide band nonselective high reflectivity and can be used as an efficient reflector to reduce solar heating.

Professor Satyendra Nath Bose

The Physics Department is one of the founding departments of the University of Dhaka which has started its long and glorious journey in 1921. Prof. S.N. Bose started his career as a teacher in this department and proposed the world-famous Bose-Einstein statistics. In 1924, the monumental work of S. N. Bose was translated by Albert Einstein to German for Zeitschrift für Physik paved the way to the formulation of quantum statistics, one of the pillars of modern physics. With this profoundly important discovery, Bose wrote the law that governs the statistics of the most abundant particles in the Universe, the bosons. Bose's work has etched the name of the Department of Physics and that of the University of Dhaka in the annals of Physics and for that matter in the history of science. In addition to theoretical research, Bose concentrated on the development of infrastructure for scientific research.