

# MD. RAKIB HOSSAIN

Dept. of Physics, BSMRSTU, Gopalganj-8100, Bangladesh  
Nationality: Bangladeshi  
Gender: Male  
Date of Birth: 22 August, 1991

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## *Research Interest*

**Computational Materials Science** (Low-dimensional nanomaterials, Density Functional Theory)

## *Education*

### **Ph.D. in Materials Science and Engineering**

August 2023 – Present

- University of Florida – USA

### **M.S. in Physics**

April 2016 – January 2018

- GPA: 3.93 out of 4
- Thesis Title: First-principles Study of Metal and Transition Metal Doped Borophene Nanocluster and Their Application as Gas Sensor
- Jahangirnagar University – Bangladesh

### **B.Sc. (Honors) in Physics**

January 2011 – March 2016

- CGPA: 3.69 out of 4
- Jahangirnagar University – Bangladesh

## *Selected Publications*

**Journal Articles: 14 (Q1 Journal – 4, Q2 Journal - 3), Total Citations – 388 (till July 2023)**

1. **Md Rakib Hossain**, Md Mehade Hasan, Maliha Nishat, Farid Ahmed, Tahmina Ferdous, Md Abul Hossain; DFT and QTAIM investigations of the adsorption of chlormethine anticancer drug on the exterior surface of pristine and transition metal functionalized boron nitride fullerene. *J. Mol. Liq.* 323, 114627 (2021).
2. **Md Rakib Hossain**, Md Mehade Hasan, Hamidur Rahman, Mohammad Sadiqur Rahman, Farid Ahmed, Tahmina Ferdous, Md Abul Hossain; Adsorption behaviour of metronidazole drug molecule on the surface of hydrogenated graphene, boron nitride and boron carbide nanosheets in gaseous and aqueous medium: A comparative DFT and QTAIM insight. *Phys. E Low-dimensional Syst. Nanostructures* 126, 114483 (2021).
3. Maliha Nishat, Md Kamal Hossain, **Md Rakib Hossain**, Shamima Khanom, Farid Ahmed, Md Abul Hossain; Role of metal and anions in organo-metal halide perovskites  $\text{CH}_3\text{NH}_3\text{MX}_3$  (M: Cu, Zn, Ga,

- Ge, Sn, Pb; X: Cl, Br, I) on structural and optoelectronic properties for photovoltaic applications; *RSC Adv.*, 12, 13281-13294 (2022).
4. Siraj Ud Daula Shamim, Md Helal Miah, **Md Rakib Hossain**, Md Mehade Hasan, Md Kamal Hossain, Md Abul Hossain, Farid Ahmed; Theoretical investigation of emodin conjugated doped B<sub>12</sub>N<sub>12</sub> nanocage by means of DFT, QTAIM and PCM analysis. *Phys. E Low-dimensional Syst. Nanostructures* 136, 115027 (2022).
  5. Md Helal Miah, **Md Rakib Hossain**, Md Saiful Islam, Tahmina Ferdous, Farid Ahmed; A theoretical study of allopurinol drug sensing by carbon and boron nitride nanostructures: DFT, QTAIM, RDG, NBO and PCM insights. *RSC Adv.* **11**, 38457–38472 (2021).
  6. Hamidur Rahman, **Md Rakib Hossain**, Tahmina Ferdous; The recent advancement of low-dimensional nanostructured materials for drug delivery and drug sensing application: A brief review. *J. Mol. Liq.* 320-A, 114427 (2020).
  7. Md Arafat Hossain, **Md Rakib Hossain**, Md Kamal Hossain, Jahirul Islam Khandaker, Farid Ahmed, Tahmina Ferdous, Md Abul Hossain; An ab-initio Study of the B<sub>35</sub> Boron Nanocluster for Application as Atmospheric Gas (NO,NO<sub>2</sub>,N<sub>2</sub>O,NH<sub>3</sub>) Sensor. *Chem. Phys. Lett.* 754, 137701 (2020).

### Conference Articles

1. Hossain, M. R. et al. Structural, electronic and optical properties of pristine and metal (Tl) doped B<sub>6</sub> nanocluster: A DFT study. in 5th IEEE Region 10 Humanitarian Technology Conference 2017, IEEE Xplore, 209–212 (2018).
2. Hossain, R. et al. The planar B<sub>6</sub> cluster as a motif for doping metal cation ( Al<sup>3+</sup> ): A DFT study. 2017 2nd Int. Conf. Electr. Electron. Eng., IEEE Xplore, 1–4 (2017).

### Conference Presentations

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#### 5<sup>th</sup> IEEE Region 10 Humanitarian Technology Conference 2017 – BUET, Bangladesh

- Structural, electronic and optical properties of pristine and metal (Tl) doped B<sub>6</sub> nanocluster: A DFT study

#### 2<sup>nd</sup> International Conference on Electrical & Electronic Engineering 2017 – RUET, Bangladesh

- The planar B<sub>6</sub> cluster as a motif for doping metal cation ( Al<sup>3+</sup> ): A DFT study

### Research Experiences

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#### Ph.D. Research Student

August 2023 – Present

- Research Project: First-principles study of functional materials
- Supervisor: Professor Dr. Simon R. Phillpot

- University of Florida – USA

**M.S. Research Student**

April 2016 – January 2018

- Research Project: First-principles study of Structural, Electronic and Optical Property of Boron Nanocluster and their applications
- Supervisor: Professor Dr. Md. Abul Hossain
- Jahangirnagar University – Bangladesh

### *Teaching Experiences*

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**Assistant Professor of Physics, Bangabandhu Sheikh Mujibur Rahman Science and Technology University, Bangladesh**

May 2021 – Present

- Conducting classes (Offered Courses: Atomic and Molecular Physics - PHY307, Health & Medical Physics – PHY455), Lab sessions (Physics Lab III) Tutorial session, Grading exam papers, proctoring exams etc.

**Lecturer of Physics, Bangabandhu Sheikh Mujibur Rahman Science and Technology University, Bangladesh**

November 2018 – April 2021

- Conducting classes (Offered Courses: Atomic and Molecular Physics - PHY307, Statistical Mechanics - PHY205, Electricity and Magnetism - PHY235); Lab sessions (Physics Lab III, Physics Minor Lab) Tutorial session, Grading exam papers, proctoring exams etc.

**Lecturer of Physics, Daffodil International University, Bangladesh**

May 2018 – November 2018

- Conducting classes (Offered Courses: Mechanics, Heat and Thermodynamics, Optics, Electricity and Magnetism)

### *Language Proficiency*

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**International English Language Testing System (IELTS)**

- Overall Band: 7.0 (Listening - 8.5, Reading – 7.0, Writing – 6.0, Speaking – 6.0)

### *Technical Skills*

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**Language/Scripts:** C++ (Basic), MATLAB (Basic), LaTeX, Origin, Mendeley

**Programs:** Gaussian 09, Adsorption Locator, CASTEP, VMD, Multiwfn, AIMALL

**Experimental Technique:** UV-Vis Spectrometer, Spin Coating Technique

## *Awards & Honors*

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Yearly university scholarship for merit	2012 – 2015
Complementary scholarship for extraordinary academic performance in all four years of undergraduate studies	2015
National Science & Technology fellowship under Ministry of Science & Technology-Government of the People's Republic of Bangladesh	2015 – 2016

## *References*

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### **Professor Dr. Tahmina Ferdous** (M.Phil. Supervisor)

Affiliation: Dept. of Physics, Jahangirnagar University, Savar, Dhaka-1342, Bangladesh.

Email: tahminaferdous1960@juniv.edu

### **Professor Dr. Md. Abul Hossain** (M.S. Supervisor)

Affiliation: Dept. of Physics, Jahangirnagar University, Savar, Dhaka-1342, Bangladesh.

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