Pranab Sarker
Postdoctoral Research Associate

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Google Scholar | LinkedIn
ResearchGate | GitHub

Personal Profile

- Ph.D. in Solid-State Physics with 10+ years of experience in ab-initio materials modeling
- 3 years of experience in ab initio and reactive molecular dynamics simulations
- 2 years of experience in coarse-grained molecular dynamics simulations of biomolecules
- Adept at postprocessing large datasets using object-oriented programming in python
- Familiar with machine-learning approaches

Research Expertise

- DFT/quantum chemistry
- Multiscale molecular dynamics
- Statistical analysis
- Materials design & screening
- Materials characterization
- Free energy calculation
- Bio-nano interface
- Zwitterionic hydration
- Scientific programming

Technical Skills

- **Simulation packages**: VASP, Quantum ESPRESSO, psi4, Gaussian, LAMMPS, and GROMACS
- **Visualization software**: Xmgrace, Matplotlib, VESTA, Avogadro, and VMD
- **Programming**: Bash, Python, and C++

Research Experience

2019 – present **Postdoctoral Researcher | Howard University & Winston-Salem State University**

Role outline: To understand (i) zwitterionic hydration/antibiofouling and (ii) protein–nanoparticles interactions
Achievements

- Elucidated the role of spacer on zwitterionic hydration/antibiofouling
- Shed light on the origin of TMAO-zwitterion's salt-resistant hydration employing *ab initio* MD
- Demonstrated how interfacial water governs peptides' adsorption on Ag-nanoparticles via coarse-grained MD
- Publications: 3 (first-author: 1; co-author: 2, *JACS*) | in-progress: 1 (first-author)

2016 – 2019 **Postdoctoral Researcher | Duke University**

Role outline: To predict synthesizable high-entropy carbides from *ab initio* high-throughput calculations
Achievements

- Formulated an *ab initio* high-throughput entropy descriptor
- Predicted 5-metal high-entropy carbides, guiding their systematic and accelerated discovery
- Publications: 3 (1 first-author: 1, *Nature Communication*)

2010 – 2015 **Ph.D. Researcher | The University of Texas at Arlington**

Role outline: To develop a pathway for efficient predictions of affordable PV and PEC solar absorbers
Achievements

- Designed and predicted W-oxides for affordable PV and PEC solar absorbers using DFT
- Developed methods for crystal structure and high-efficiency thermodynamic growth conditions predictions
- Publications: 13 (first-author: 5)

Education

- **2010 - 2015** **Ph.D. in Physics** (The University of Texas at Arlington, USA)
- **2008 - 2009** **M.Sc. in Physics** (University of Dhaka, Bangladesh)
- **2002 - 2008** **B.Sc. in Physics** (University of Dhaka, Bangladesh)

AWARDS & NEWS

- APS Energy Research Workshop Program travel grant, 2022 & 2013, recipient
- Richard Jack Marquies Physics Scholarship, 2015, recipient
- Duke University: *Disordered Materials Could Be Hardest, Most Heat-Tolerant Ever*
- Chemistry World: *New class of carbides could be toughest yet*

Personal Development

- Deep Learning: Artificial Neural Networks (Udemy online courses)

Scholarly Services

- Journal referee: The Journal of Physical Chemistry, ACS Omega, Journal of Materials Research, and Computer Physics Communications

Professional Affiliations

- APS, ACS, AIChE, and MRS

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Selected Publications

[1] **P. Sarker** and M. N. Huda, "Determination of thermodynamic growth conditions for a high-efficiency $Cu_2ZnSn(S_{1-x}Se_x)_4$", Comput. Mater. Sci. **208**, (111313) (2022).

[2] **P. Sarker***, M. S. J. Sajib*, X. Tao, and T. Wei, "Multiscale simulation of protein corona formation on silver nanoparticles: study of ovispirin-1 peptide adsorption (* = contributed equally)", J. Phys. Chem. B **126**, 601 (2022).

[3] **P. Sarker**, T. Harrington*, C. Toher, C. Oses, M. Samiee, J.-P. Maria, D. W. Brenner, K. S. Vecchio, and S. Curtarolo, "High-entropy high-hardness metal carbides discovered by entropy descriptors (* = contributed equally)", Nat. Commun. **9**, 4980 (2018).

[4] **P. Sarker** and M. N. Huda, "Understanding the thermodynamic pathways of SnO-to-SnO_x phase transition", Comput. Mater. Sci. **111**, 359 (2016).

[5] **P. Sarker**, M. M. Al-Jassim, and M. N. Huda, "Predicting a quaternary tungsten oxide for sustainable photovoltaic application by density functional theory", Appl. Phys. Lett. **107**, 233902 (2015).

[6] **P. Sarker**, M. M. Al-Jassim, and M. N. Huda, "Theoretical limits on the stability of single-phase kesterite-Cu_2ZnSnS_4", J. Appl. Phys. **117**, 035702 (2015).

[7] **P. Sarker**, D. Prasher, N. Gaillard, and M. N. Huda, "Predicting a new photocatalyst and its electronic properties by density functional theory", J. Appl. Phys. **114**, 133508 (2013).

[8] H. Huang, C. Zhang, R. Crisci, H.-C. Hung, T. Lu, H.-C. Hung, M. S. J. Sajib, **P. Sarker**, J. Ma, T. Wei, S. Jiang, and Z. Chen, "Strong surface hydration and salt resistance mechanism of a new zwitterionic polymer based on protein stabilizer TMAO", J. Am. Chem. Soc. (2021) `10.1021/jacs.1c08280`.

[9] M. S. J. Sajib, **P. Sarker**, Y. Wei, X. Tao, and T. Wei, "Protein corona on gold nanoparticles studied with hybrid coarse-grained and atomistic simulations", Langmuir **36**, 13356–13363 (2020).

[10] Z. Zhu, **P. Sarker**, C. Zhao, L. Zhou, R. L. Grimm, M. N. Huda, and P. M. Rao, "Photoelectrochemical properties and behavior of α-$SnWO_4$ photoanodes synthesized by hydrothermal conversion of WO_3 films", ACS Appl. Mater. Interfaces **9**, 1459 (2017).

[11] G. Sharma, Z. Zhao, **P. Sarker**, B. A. Nail, J. Wang, M. N. Huda, and F. E. Osterloh, "Electronic structure, photovoltage, and photocatalytic hydrogen evolution with p-$CuBi_2O_4$ nanocrystals", J. Mater. Chem. A **4**, 2936 (2016).

Selected Conference and Workshop Talks

[1] **P**. Sarker and T. Wei. Understanding strong hydration, salt-resistance, and antibiofouling of zwitterionic materials from ab initio simulations, APS March Meeting, 2022.

[2] **P. Sarker**, Md S. J. Sajib, T. Wei, Quantum and atomistic molecular dynamics simulations of zwitterionic TMAO's hydration and anti-biofouling, ACS Spring Meeting, 2021.

[3] **P. Sarker**, Electronic Structure Simulation, BioNano Workshop, Howard University, 2020.

[4] **P. Sarker**, C. Toher, T. Harrington, J. Gild, J. Luo, J.-P. Maria, D. Brenner, K. Vecchio, and S. Curtarolo, Formulation of an entropy descriptor for entropy stabilized compounds from high-throughput DFT, APS March Meeting, 2017.

[5] **P. Sarker** and M. N. Huda, Theoretical study on single-phase stability and intrinsic defects in different $Cu_2ZnSn(Se_{1-x}S_x)_4$ alloys, APS March Meeting, 2015.

[6] **P. Sarker**, T. J. Harrison, M. M. Al-Jassim, and M. N. Huda, Theoretical study on the growth conditions for single-phase stability of kesterite-Cu_2ZnSnS_4, APS March Meeting, 2014.

[7] **P. Sarker** and M. N. Huda, Predicting a new quaternary metal oxide and the study of its structural, electronic, and optical properties by density functional theory, APS March Meeting, 2013.

[8] **P. Sarker** and M. N. Huda, Determination of crystal structure and the study of electronic properties of $AgBiW_2O_8$ by density functional theory, APS March Meeting, 2012.

Selected Conference and Workshop Posters

[1] **P. Sarker**, M. S. J. Sajib, and T. Wei. Analysis of the zwitterionic hydration and antibiofouling using quantum and atomistic simulations (the most exceptional abstract submitted to Division of Computers in Chemistry), Sci-Mix session, ACS Fall Meeting, 2021.

[2] **P. Sarker**, M. M. Al-Jassim, and M. N. Huda, Determination of single-phase stability of a defect induced multi-cation material, The Annual Workshop on Recent Developments in Electronic Structure Theory, 2014.