Pranab Sarker

Scientist

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Department of Biomedical Engineering
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Google Scholar ResearchGate Web

Education

Ph.D. 2010 – 2015 Theoretical Condensed Matter Physics, The University of Texas at Arlington, USA
Dissertation: *Theoretical Prediction of Materials for Efficient Conversion of Solar Energy*
Advisor: Muhammad N. Huda, Ph.D.

B.Sc. 2002 – 2008 Physics, University of Dhaka, Bangladesh

Research Experience—Scientist and Postdoctoral Research Associate

09/2023 – present Scientist, Department of Biomedical Engineering, University of South Carolina (USC)
07/2021 – 08/2023 Postdoc, Department of Chemical Engineering, Howard University (HU), USA
07/2020 – 06/2021 Postdoc, Department of Chemical Engineering, Howard University (HU)
07/2019 – 06/2020 Postdoc, Department of Chemistry, Winston-Salem State University (WSSU)
03/2016 – 05/2019 Postdoc, Department of Mechanical Engineering and Materials Science, Duke University

Research Interests

My research interests include chiroptical properties of 2D-chiral hybrid halide perovskites, hydration and antibiofouling of zwitterion, protein-nanoparticle interaction, solar energy conversion (PV/PEC), and high-entropy ceramics—with a focus on *ab initio* materials design and multiscale modeling.

Research Accomplishments

- Publications: 27 (9 as a first author) | citations: 2200+ | h-index: 14 | i10-index: 15
- Demonstrated how a chiral-achiral cation mixing enhances CD in 2D-chiral hybrid halide perovskites
- Established a structure-property (CD) correlation in 2D-chiral hybrid halide perovskites
- Revealed how the charge separation of a zwitterion controls its hydration and antibiofouling efficacy
- Shed light on the origin of antibiofouling efficacy of TMAO molecule and TMAO-derived polymer surfaces
- Provided insights into the interfacial hydration effects on protein adsorption on nanoparticles
- Developed an *ab initio* high-throughput entropy descriptor to identify synthesizable high-entropy carbides
- Rationally designed $CuBiW_2O_8$ and $CuSnW_2O_8$ for PEC and PV, respectively
- Explained the multiphase formation of Cu_2SnZnS_4 and its alloy, $Cu_2SnZn(S_{1-x},Se_x)_4$
- Elucidated the underlying mechanism in the SnO-to-SnO_x ($1 < x \leq 2$) phase transition
- Identified defects that primarily limit $CuBi_2O_4$'s and SnW_2O_4's photocatalytic (PEC) performances

Proposal Experience

- PI, 1,500,000 ACCESS Discover High-Performance Computing (HPC) credits (MAT230079) (awarded)
  Project: *Atomistic Simulations of 2D-Chiral Organic-Inorganic Hybrid Halide Perovskites*
- Participated in an NSF-EPM proposal writing (submitted)

Teaching

2010 – 2015 **Enhanced Graduate Teaching Assistant**, Dept. of Physics, University of Texas at Arlington, USA
Labs taught: Modern Physics (PHYS 3183); Mechanics & Sound and Electricity & Light (PHYS 1441-1444); and Sound, Light, Electricity, and Magnetism (PHYS 1301-1302)

2010 **Physics Lecturer**, Dept. of Civil Engineering, Presidency University, Dhaka, Bangladesh
Courses taught: Physical Optics, Heat & Thermodynamics, and Waves & Oscillations (PHYS 101); and Structure Matter, Electricity & Magnetism, and Modern Physics (PHYS 103)

Awards

- 2022 & 2013 Travel grant, APS energy research workshop program
- 2015 Richard Jack Marquies physics scholarship, The University of Texas at Arlington

Publications

Submitted papers

1. Z. Gandhi, T. Lu, W. Guo, R. Crisci, J. Gao, M. C. Wilson, C. R. So, **P. Sarker**, X. Qin, T. Wei, and Z. Chen, Probing molecular interactions between barnacle peptides and polymers in situ to understand bioadhesion, Angew. Chem. **under review** (2024).

Refereed papers (* = contributed equally; † = corresponding author)

1. X. Qin, A. Chen, J. Fang, **P. Sarker**, M. J. Uline, and T. Wei, Hydration and antibiofouling behavior of amphiphilic polymer brush surfaces functionalized with TMAO and short fluorocarbon: a study with atomistic molecular dynamics simulations, Langmuir **accepted** (2024) 10.1021/acs.langmuir.4c03218.
2. H. Li, **P. Sarker**, X. Zhang, M. W. Terban, S. Ghose, I. Dursun, M. Cotlet, M. Li, Y. Zhang, Y. Xu, S. Ramakrishnan, T. Wei, D. Lu, and Q. Yu, Enhancing chiroptoelectronic activity in chiral 2D perovskites via chiral-achiral cation mixing, Adv. Opt. Mater. **accepted** (2024) 10.1002/adom.202401782.
3. C. A. Psarakis, T. T. Fidelis, K. B. Chin, B. Journaux, A. Kavner, **P. Sarker**, M. J. Styczinski, S. D. Vance, and T. Wei, Electrical conductivity of subsurface ocean analogue solutions from molecular dynamics simulations, ACS Earth Space Chem. **8**, 1146–1153 (2024).
4. Y. Wu, T. Lin, E. Santos, D. Ahn, R. Marson, **P. Sarker**, X. Chen, F. Gubbels, N. E. Shephard, C. Mohler, T. Wei, T.-C. Kuo, and Z. Chen, Molecular behavior of silicone adhesive at buried polymer interface studied by molecular dynamics simulation and sum frequency generation vibrational spectroscopy, Soft Matter **20**, 4765–4775 (2024).
5. I. Dursun, M. Terban, Y. Xu, X. Zhang, S. Ghose, M. Li, **P. Sarker**, H. Li, M. Cotlet, T. Wei, D. Lu, and Q. Yu, Temperature-dependent optical and structural properties of chiral two-dimensional hybrid lead-iodide perovskites, J. Phys. Chem. C **127**, 15423–15434 (2023).
6. **P. Sarker**, T. Lu, D. Liu, G. Wu, H. Chen, M. S. J. Sajib, S. Jiang, Z. Chen, and T. Wei, Hydration behaviors of nonfouling zwitterionic materials **(selected for the 2023 Chemical Science HOT Article Collection)**, Chem. Sci. **14**, 7500–7511 (2023).
7. G. T. Chen, **P. Sarker**†, B. Qiao, and T. Wei, Mesoscopic simulations of protein corona formation on zwitterionic peptide-grafted gold nanoparticles, J. Nanopart. Res. **25**, 108 (2023).
8. Z. Yuan, P. McMullen, S. Luozhong, **P. Sarker**, C. Tang, T. Wei, and S. Jiang, Hidden hydrophobicity impacts polymer immunogenicity, Chem. Sci. **14**, 2033–2039 (2023).
9. **P. Sarker**, G. Chen, M. S. J. Sajib, N. W. Jones, and T. Wei, Hydration and antibiofouling of TMAO-derived zwitterionic polymers surfaces studied with atomistic molecular dynamics simulations, Colloid. Surf. A-Physicochem. Eng. Asp. **653**, 129943 (2022).
10. **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).
11. **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, J. Phys. Chem. B **126**, 601 (2022).
12. 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. **143**, 16786 (2021).
13. 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 (2020).
14. T. J. Harrington, J. Gild, **P. Sarker**, C. Toher, C. M. Rost, O. F. Dippo, C. McElfresh, K. Kaufmann, E. Marin, L. Borowski, P. E. Hopkins, J. Luo, S. Curtarolo, D. W. Brenner, and K. S. Vecchio, Phase stability and mechanical properties of novel high entropy transition metal carbides, Acta Mater. **166**, 271–280 (2019).
15. **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, Nat. Commun. **9**, 4980 (2018).
16. Z. Rak, C. M. Rost, M. Lim, **P. Sarker**, C. Toher, S. Curtarolo, J.-P. Maria, and D. W. Brenner, Charge compensation and electrostatic transferability in three entropy-stabilized oxides: results from density functional theory calculations, J. Appl. Phys. **120**, 095105 (2016).
17. 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).

18. A. Kormányos, A. Thomas, M. N. Huda, **P. Sarker**, J. P. Liu, N. Poudyal, C. Janáky, and K. Rajeshwar, Solution combustion synthesis, characterization, and photoelectrochemistry of $CuNb_2O_6$ and $ZnNb_2O_6$ nanoparticles, J. Phys. Chem. C **120**, 16024 (2016).
19. 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).
20. **P. Sarker** and M. N. Huda, Understanding the thermodynamic pathways of SnO-to-SnO_x phase transition, Comput. Mater. Sci. **111**, 359 (2016).
21. **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).
22. A. Thomas, C. Janáky, G. F. Samu, M. N. Huda, **P. Sarker**, J. P. Liu, V. van Nguyen, E. H. Wang, K. A. Schug, and K. Rajeshwar, Time- and energy-efficient solution combustion synthesis of binary metal tungstate nanoparticles with enhanced photocatalytic activity, ChemSusChem **8**, 1652 (2015).
23. **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).
24. **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).
25. M. N. Huda, T. G. Deutsch, **P. Sarker**, and J. A. Turner, Electronic structure study of N,O related defects in GaP for photoelectrochemical applications, J. Mater. Chem. A **1**, 8425 (2013).
26. N. R. de Tacconi, H. K. Timmaji, W. Chanmanee, M. N. Huda, P. **Sarker**, C. Janáky, and K. Rajeshwar, Photocatalytic generation of syngas using combustion-synthesized silver bismuth tungstate, ChemPhysChem **13**, 2945 (2012).

Papers in refereed conference proceedings

1. D. Prasher, M. Chong, Y. Chang, **P. Sarker**, M. N. Huda, and N. Gaillard, Development of metal tungstate alloys for photoelectrochemical water splitting, Proc. SPIE **8822**, 8822 (2013).

Unpublished working papers

1. X. Qin, J. Fang, R. Gambarini, **P. Sarker**, C. Tang, M. J. Uline, and T. Wei, Antimicrobial behavior of facial amphiphilic materials studied with atomistic molecular dynamics simulations (in prep.) (2024).

Selected Research Presentations

Talks: Invited

- **P. Sarker**. Multidisciplinary Computational Materials Research: Antibiofouling Zwitterions And 2D Achiral-Chiral Hybrid Halide perovskites. Department of Physics, Howard University, 2023.
- **P. Sarker**. Materials Design and Characterization Using Multiscale Modelling. Global Congress on Materials Science and Engineering (GCMSE2023), 2023.

Talks: Contributed

- **P. Sarker**, Hao Li, Deyu Lu, Tao Wei, and Qiuming Yu, Unraveling the origin of chiroptical properties in 2D achiral-chiral hybrid lead perovskites from first-principles calculations, APS March Meeting, 2023.
- **P. Sarker**, Grace Tang Chen, Md Symon Jahan Sajib, Nathan Wesley Jones, and Tao Wei. Atomistic modeling of hydration and antibiofouling of TMAO-polymer surfaces, APS March Meeting, 2023.
- **P. Sarker** and T. Wei. Understanding strong hydration, salt-resistance, and antibiofouling of zwitterionic materials from ab initio simulations, APS March Meeting, 2022.
- **P. Sarker**, M. S. J. Sajib, and T. Wei. Understanding the zwitterionic hydration from ab initio simulations, MRS Fall Meeting & Exhibit, 2021.
- **P. Sarker**, M. S. J. Sajib, and T. Wei. Ab initio molecular dynamics simulations of the hydration of zwitterions, AIChE Annual Meeting, 2021.
- **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 the Division of Computers in Chemistry), ACS Fall Meeting, 2021.
- **P. Sarker**, M. S. J. Sajib, and T. Wei. Quantum and atomistic molecular dynamics simulations of zwitterionic TMAO's hydration and anti-biofouling, ACS Spring Meeting, 2021.

- **P. Sarker**. Electronic structure simulations: From materials discovery to characterization, BioNano Workshop, Howard University, 2021.
- **P. Sarker**. Electronic structure simulations, BioNano Workshop, Howard University, 2020.
- **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.
- **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.
- **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.
- **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.

Posters: Conferences and Workshops

- J. R. Stevenson, **P. Sarker**, M. Moss, and T. Wei. Peptoids as RAGE antagonists: Simulating new treatments for Alzheimer's (2nd best poster award), Research Symposium, University of South Carolina, 2023.
- **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 the Division of Computers in Chemistry), Sci-Mix session, ACS Fall Meeting, 2021.
- **P. Sarker**, T. Harrington, C. Toher, C. Oses, J. Gild, C. M. Rost, O. F. Dippo, M. Samiee, J. Luo, J.-P. Maria, D. W. Brenner, K. Vecchio, and S. Curtarolo. Entropy forming ability and beyond, The Annual Funding Review in the Multidisciplinary University Research Initiatives, 2018.
- **P. Sarker**, C. Toher, T. Harrington, J. Gild, J. Luo, J.-P. Maria, D. Brenner, K. Vecchio, and S. Curtarolo. Entropy Descriptors From High-throughput DFT, The Annual Funding Review in the Multidisciplinary University Research Initiatives, 2016.
- **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.

Mentoring

Graduate Students

2023 - present	**Yuchen Wu**, Department of Chemistry, University of Michigan, USA
2021 - 2022	**Fidelis Timothy Tizhe**, Department of Chemical Engineering, Howard University, USA

Undergraduate Students

2023 (Summer)	**Jack StevensonJack**, Department of Computer Science, Oregon State University, USA
2023 (Summer)	**Monique Fletcher**, Department of Chemical Engineering, Howard University, USA
2019 - 2021	**Maurice O. Biggers**, Department of Chemistry, Winston-Salem State University, USA
2019 - 2020	**Joselyn Sixtos-Aguirre**, Division of Nursing, Winston-Salem State University, USA
	Samuel E. Chance, Department of Computer Science, Winston-Salem State University, USA
2012 - 2014	**Tyler Harrison**, Department of Physics, University of Texas at Arlington, USA

High School Students

2022	**Grace Chen**, Adlai E. Stevenson High School, Lincolnshire, IL, USA

Professional Activities

- **Journal referee**: Langmuir, Soft Matter, ACS Applied Energy Materials, The Journal of Physical Chemistry, ACS Omega, Journal of Materials Research, Computer Physics Communications, Colloids and Surfaces B: Biointerfaces, Nanomaterials, Entropy, Metals, Journal of Composites Science, Materials, and Coatings

Membership of Associations

- American Physical Society (APS), American Chemical Society (ACS), American Institute of Chemical Engineers (AICheE), and Materials Research Society (MRS)

Press and News Releases

- University of South Carolina, 06/21/2024: *ONR-sponsored research aims to eliminate biofouling on naval vessels*
- Duke University, 11/26/2018: *Disordered Materials Could Be Hardest, Most Heat-Tolerant Ever*
- Chemistry World, 12/03/2018: *New class of carbides could be toughest yet*

Skills

Computation

- Software: VASP, Quantum ESPRESSO, FHI-AIMS, Gaussian, Psi4, Q-Chem, ORCA, GROMACS, and LAMMPS
- Methods: DFT, DFPT, SAPT, QTAIM, *Ab initio* MD, Reactive MD, classical MD, and coarse-grained MD
- High-throughput framework: AFLOW

Post-Processing and Data Analysis

- Programming Languages: Bash, C++, Python, and Git

Visualization

- Data: Xmgrace and gnuplot
- Electronic/crystallographic/trajectory analysis: VESTA, Avogadro, GaussView, IQmol, and VMD

Documentation and Presentation

- LaTeX and Microsoft Office—Word, Excel, and PowerPoint