

Pranab Sarker

Scientist

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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 Chemical Engineering, University of South Carolina (USC), USA
- 07/2021 – 08/2023 Postdoc, Department of Chemical Engineering, Howard University (HU), USA
Project 1: *Developing antibiofouling and fouling release materials/surfaces*
Advisor: Tao Wei, Ph.D. (USC & HU)
Project 2: *Experimental and Theoretical Investigation of Phase-Pure and Orientation Controlled Two-Dimensional (2D) Ruddlesden-Popper Metal-Halide Perovskites*
Advisors: Qiuming Yu, Ph.D. (Cornell University), Deyu Lu, Ph.D. (Brookhaven National Lab), and Tao Wei, Ph.D. (USC & HU)
- 07/2020 – 06/2021 Postdoc, Department of Chemical Engineering, Howard University (HU), USA
- 07/2019 – 06/2020 Postdoc, Department of Chemistry, Winston-Salem State University (WSSU), USA
Joint Project: *Understanding Interactions of Gold and Silver nanoparticles with Proteins to Achieve Optimum Surface Plasmon Effect*
Advisors: Tao Wei, Ph.D. (HU) and Xiuping Tao, Ph.D. (WSSU)
- 03/2016 – 05/2019 Postdoc, Department of Mechanical Engineering and Materials Science, Duke University, USA
Project: *Entropy-Stabilized Ultra-High Temperature Ceramics*
Advisor: Stefano Curtarolo, Ph.D.

Research Interests

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

Research Accomplishments

- Publications: 23 (9 as a first author) | citations: 1700+ | h-index: 13 | i10-index: 13
- Revealed how the zwitterionic charge separation 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
- Unraveled the chiroptical properties in 2D-chiral-achiral hybrid halide perovskites
- Developed an *ab initio* high-throughput entropy descriptor to identify synthesizable high-entropy carbides
- Rationally designed tungstate-based affordable PV/PEC materials for renewable energy applications
- Developed a framework to predict the thermodynamic phase-stability/optimal growth conditions:
 - Explained the multiphase formation of CZTS
 - Predicted thermodynamic growth conditions of CZTSSe to obtain its high PV efficiency
 - Elucidated the thermodynamic pathways of SnO-to-SnO_x ($1 < x \leq 2$) phase transition

Teaching

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

Awards

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

Publications

Refereed research papers (Total: 22)

1. 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).
2. **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).
3. G. T. Chen, **P. Sarker**[†], B. Qiao, and T. Wei, Mesoscopic simulations of protein corona formation on zwitterionic peptide-grafted gold nanoparticles ([†] = corresponding author), *J. Nanopart. Res.* **25**, 108 (2023).
4. 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).
5. **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).
6. **P. Sarker**[†] and M. N. Huda, Determination of thermodynamic growth conditions for a high-efficiency $\text{Cu}_2\text{ZnSn}(\text{S}_{1-x}\text{Se}_x)_4$ ([†] = corresponding author), *Comput. Mater. Sci.* **208**, (111313) (2022).
7. **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).
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.* **143**, 16786 (2021).
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 (2020).
10. 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).
11. **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).
12. 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).
13. Z. Zhu^{*}, **P. Sarker**^{*}, C. Zhao, L. Zhou, R. L. Grimm, M. N. Huda, and P. M. Rao, Photoelectrochemical properties and behavior of $\alpha\text{-SnWO}_4$ photoanodes synthesized by hydrothermal conversion of WO_3 films (^{*} = contributed equally), *ACS Appl. Mater. Interfaces* **9**, 1459 (2017).
14. 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).
15. 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).
16. **P. Sarker** and M. N. Huda, Understanding the thermodynamic pathways of SnO -to- SnO_x phase transition, *Comput. Mater. Sci.* **111**, 359 (2016).
17. **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).
18. 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).
19. **P. Sarker**, M. M. Al-Jassim, and M. N. Huda, Theoretical limits on the stability of single-phase kesterite- $\text{Cu}_2\text{ZnSnS}_4$, *J. Appl. Phys.* **117**, 035702 (2015).
20. **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).
21. 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).

22. 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. H. Li, P. Sarker, X. Zhang, S. Ghose, I. Dursun, D. Lu, M. Cotlet, M. Li, Y. Zhang, Y. Xu, S. Ramakrishnan, T. Wei, and Q. Yu, Manipulating the chirality in 2D hybrid lead perovskites via achiral cations (in prep.) (2023).
2. Y. Wu, T. Lin, E. Santos, D. Ahn, R. Marson, P. Sarker, X. Chen, G. Frederic, C. Tucker, N. E. Shephard, C. Mohler, T. Wei, T.-C. Kuo, and Z. Chen, Molecular behavior of adhesion promoter in silicone adhesive at buried polymer interface studied by molecular dynamics simulation and sum frequency generation vibrational spectroscopy, (2023).
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 analog solutions from molecular dynamics simulations (in prep.) (2023).

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 $\text{Cu}_2\text{ZnSn}(\text{Se}_{1-x}\text{S}_x)_4$ 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- $\text{Cu}_2\text{ZnSnS}_4$, 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

- **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

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|----------------|---|
| 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

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|---------------|---|
| 2023 (Summer) | Jack StevensonJack , Department of Computer Science, Oregon State 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

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| 2022 | Grace Chen , Adlai E. Stevenson High School, Lincolnshire, IL, USA |
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Professional Activities

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

Membership of Associations

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

Press and News Releases

- 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