Pranab Sarker

Postdoctoral Research Associate

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Department of Chemical Engineering
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Employment

Postdoctoral Research Associate

07/2020 – present Department of Chemical Engineering, Howard University (HU), USA
07/2019 – 06/2020 Department of Chemistry, Winston-Salem State University (WSSU), USA
03/2016 – 05/2019 Department of Mechanical Engineering and Materials Science, Duke University, USA

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*

M.Sc. 2008 – 2009 Theoretical Condensed Matter Physics, University of Dhaka, Bangladesh
Thesis: *A Theoretical Study of Surface Tension of Crude Oil*

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

Research

My research covers various topics and interests—bio-nano interface, zwitterionic antibiofouling, solar energy conversion (PV/PEC), 2D-chiral hybrid perovskites, and ultra-high temperature ceramics—with a focus on *ab initio* materials design and multiscale characterization.

Research Accomplishments

- Developed an *ab initio* high-throughput entropy descriptor to identify synthesizable high-entropy carbides (HECs)
- Rationally designed tungstate-based affordable PV/PEC materials for renewable energy applications
- Provided new structural insights into 2D-chiral hybrid organic-inorganic perovskites design
- Identified defects that primarily limit $CuBi_2O_4$'s and SnW_2O_4's photocatalytic (PEC) performances
- Developed a framework to predict thermodynamic phase-stability and optimal growth conditions
  - Explained the multiphase formation of PV-CZTS
  - Predicted thermodynamic growth conditions to obtain high-efficiency PV-CZTSSe
- Explored the phase-stability and optoelectronic properties of Sn_2O_3 for solar energy applications
- Shed light on the source of TMAO's strong salt-resistant antibiofouling efficacy
- Elucidated the role of spacer on zwitterionic hydration
- Demonstrated the size effect of Ag/Au nanoparticles on peptide/protein adsorption

Proposal Experience

- Contributed, Center for Transformative Materials Synthesis and Manufacturing, DOE-EFRC (DE-FOA-0002653) (Not Funded)

Awards

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

Professional Activities

- Journal referee: The Journal of Physical Chemistry, ACS Omega, Journal of Materials Research, Computer Physics Communications, and Materials Science in Semiconductor Processing
- Team member: Cyber Training on Materials Genome Innovation for Computational Software (CyberMAGICS)

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*

Publications

Refereed research papers

1. Z. Yuan, P. McMullen, S. Luozhong, **P. Sarker**, C. Tang, T. Wei, and S. Jiang, Hidden hydrophobicity impacts polymer immunogenicity, Adv. Sci. **(under review)** (2022).
2. **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).
3. **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).
4. **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).
5. 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).
6. 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).
7. 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).
8. **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).
9. 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).
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 (* = contributed equally), ACS Appl. Mater. Interfaces **9**, 1459 (2017).
11. 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).
12. 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).
13. **P. Sarker** and M. N. Huda, Understanding the thermodynamic pathways of SnO-to-SnO_x phase transition, Comput. Mater. Sci. **111**, 359 (2016).
14. **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).
15. 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).
16. **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).
17. **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).
18. 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).
19. 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. **P. Sarker**, W. Guo, H. Chen, S. Jiang, Z. Chen, and T. Wei, Hydration of zwitterions (**to be submitted to** PNAS), (2022).
2. 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, Reveal the origin of chiral optical properties in 2D hybrid lead perovskites via achiral cations (in prep.) (2022).
3. **P. Sarker**, M. S. J. Sajib, and T. Wei, Chemisorption and mobility of amino acids on Au surface (in prep.) (2022).
4. C. A. Psarakis, T. T. Fidelis, K. B. Chin, B. Journaux, A. Kavner, M. J. Styczinski, S. D. Vance, **P. Sarker**, and T. Wei, Conductivity of subsurface ocean analog solutions from molecular dynamics simulations (in prep.) (2022).

Selected Research Presentations

Talks: Invited

- **P. Sarker**. Multiscale Simulation: From Materials Design to Characterization. Global Congress on Materials Science and Engineering (GCMSE2023), 2023.

Talks: Contributed

- **P. Sarker**. Hydration, salt-resistance, and antibiofouling of zwitterionic materials, US-North Africa Conference of Nanotechnology convergence on Energy, Enviroment and Health, 2022.
- **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.
- **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.

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.

Teaching

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

2010 **Physics Lecturer**, Presidency University, Dhaka, Bangladesh
Physics courses
- PHYS 101: Physical Optics, Heat & Thermodynamics, and Waves & Oscillations
- PHYS 103: Structure Matter, Electricity & Magnetism, and Modern Physics

Physics lab
- PHYS 104: Optics, Heat & Thermodynamics, Electricity, and Mechanics

Mentoring

Graduate

2021 - 2022 **Fidelis Timothy Tizhe**, Department of Chemical Engineering, Howard University, USA

Undergraduate

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 Student

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

Skills

Computation
- Software packages: VASP, Quantum ESPRESSO, Gaussian, Psi4, LAMMPS, and GROMACS
- 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, and VMD

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