

Anusheela Das

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CURRENT POSITION

Feb 2022 - **Postdoctoral Researcher, NASA Jet Propulsion Laboratory**

EDUCATION

August 2016 - Dec 2021 **PhD, Materials Science and Engineering, Advisor – Prof. Michael Bedzyk**
Northwestern University (NU), Evanston, IL , USA
(GPA: 3.9/4)

July 2012 - July 2016 **Bachelor of Technology (Hons.), Metallurgical and Materials Engineering**
Indian Institute of Technology (IIT), Kharagpur, India
GPA: 9.25/10 (Dept. Rank 1 / 33)

AWARDS & ACHIEVEMENTS

- 2021 Final Year Fellowship from McCormick School of Engineering at NU
- 2017 Hierarchical Materials Cluster (HMCP) Fellowship at NU (for inter-disciplinary student research)
- 2016 Institute Medal for Department Rank 1, Class of 2016, IIT Kharagpur
- 2016 Usha Martin Award for best B.Tech Thesis in department, IIT Kharagpur
- 2016 Indranil Award by Metallurgical Institute of India (MGMI) for outstanding contribution in the field
- 2015 Summer Research Fellowship by Indian Academy of Sciences (IAS)
- 2014 Summer Research Fellowship by Indian Institute of Science Education and Research (IISER)
- 2012 Young Scientist Fellowship (KVPY) by Department of Science and Technology of Govt. of India
- 2011 National Merit Awardee in Mathematics Olympiad, 2011

RESEARCH EXPERIENCE

- Sept 2016 – Dec 2021
PhD thesis
- Atomic-scale structural study of functionalized metal and their oxides through surface-sensitive x-ray characterization**
Advisor: Prof. Michael Bedzyk, Dept. of MSE,, Dept. of Physics and Astronomy, NU
- Atomic layer deposition (ALD) grown thin films of VO_x, Pt, MoO_x important in semiconductor and catalysis industries
 - X-ray standing wave (XSW), X-ray photoelectron spectroscopy (XPS) and X-ray absorption spectroscopy studies (EXAFS and XANES)
 - Conducted experiments at synchrotron facilities: Advanced Photon Source, USA and Diamond Light Source, UK
- Aug. 2015 - April 2016
B. Tech thesis
- Development and characterisation of shape-memory magnetocaloric alloys for magnetic cooling: a non-conventional source of energy**
Advisor: Dr. Jayanta Das, Dept. of MME., IIT Kharagpur, India
- Analysed magnetic properties of Fe-Ni based nanocomposites with varying Ga content to obtain an alloy with near room temperature Curie temperature (T_c) for maximizing its efficiency in magnetic cooling and making it commercially viable. (*paper submitted to Prog. Nat. Sci.*)
 - Characterisation techniques : SQUID, SEM, EDS, X-ray diffraction (XRD)
- May 2015 - July 2015
Undergrad fellowship
- Study the effect of Molybdenum on plasticity in the titanium alloys**
Advisor: Prof. Dipankar Banerjee, Dept. of Materials Engineering, IISc Bangalore, India
- Devised method of slip analysis in mechanically deformed titanium alloys to determine the activated slip systems in each grain, using SEM image and EBSD scans, which helped in selection of most efficient alloy for aero-engines.
 - Characterisation techniques: Micro-indentation, nanoindentation, EPMA, SEM

May 2014 - July 2014
Undergrad fellowship

Theoretical modelling of heterogeneity in single molecule nanoparticle catalysis

Advisor: Dr. Srabanti Chaudhury, Dept. of Chemistry, IISER Pune, India

- Built a theoretical framework, based on the first passage time distribution, to calculate the catalytic reaction rates of metal nanoparticle catalysis by obtaining closed form analytical expressions for the randomness parameter, a measure of dynamic disorder in single molecule catalysis. (*paper published in Chem. Phys. Lett.*)

PUBLICATIONS

JOURNAL

- A. Das, S. Chaudhury; “Modelling the heterogeneous catalytic activity of a single nanoparticle using a first passage time distribution formalism”, *Chem. Phys. Lett.* 641, pp 193–198 (2015)
- P. Liu, Y. Zhang, C. Liu, J. Emery, A. Das, M. Bedzyk, A. Hock, A. Martinson; “Thermal Atomic Layer Deposition of Gold: Mechanistic Insights, Nucleation, and Epitaxy”, *ACS Appl. Mater. Interfaces* (2021)
- A. Das, H. Park, Y. Chen, D. Choudhury, T.L. Lee, J. Elam, P. Zapol, M. Bedzyk; “Atomic-scale structure of chemically distinct surface oxygens in redox reactions”, *J. Amer. Chem. Soc.*, (2021)
- Y. Liu, J. Li, A. Das, H. Kim, L. O. Jones, Q. Ma, M. J. Bedzyk, G. C. Schatz, Y. Kratish, T. J. Marks; “Synthesis and Structure-Activity Characterization of a Single-Site MoO₂ Catalytic Center Anchored on Reduced Graphene Oxide” *J. Amer. Chem. Soc.*, (2021)
- J. Li, A. Das, Q. Ma, M. J. Bedzyk, Y. Kratish, T. J. Marks; “Diverse Mechanistic Pathways in Single-Site Heterogeneous Catalysis. Alcohol Conversions Mediated by a High-Valent Carbon-Supported Molybdenum-Dioxo Catalyst”, *ACS Catalysis*, (2021)
- A. Das, H. Park, Y. Chen, D. Choudhury, T.L. Lee, J. Elam, P. Zapol, M. Bedzyk; “Atomic-scale view of redox induced changes for monolayer MoO_x on α -TiO₂ (110) with chemical-state sensitivity” (Prepared for submission, *J. Amer. Chem. Soc.*, 2022)
- Y. Chen, L. O. Jones, A. Das, M. A. Mosquera, T. L. Lee, D. T. Keane, G. C. Schatz, M. J. Bedzyk; “Site-specific valence band of Pt/SrTiO₃ (001) interface via X-ray standing wave excited photoelectron emission” (Under Review, *Phys. Rev. Lett.*, 2022)
- A. H. Mason, A. Motta, A. Das, Q. Ma, M. J. Bedzyk, Y. Kratish, T. J. Marks “Facile Polyolefin Plastics Hydrogenolysis Catalyzed by a Surface Electrophilic d⁰ Hydride” (Under Review, *Nature Catalysis* 2022)

CONFERENCE

- A. Das, Y. Chen, D. T. Keane, J. Rix, M. J. Bedzyk, “Atomic-scale interfacial structure studies of oxide-supported catalysts using XSW-HAXPES”, APS/CNM User Meeting, Virtual, May 2021, (Poster)
- A. Das, Y. Chen, D. Choudhury, L.O. Jones, D. T. Keane, A.U. Mane, J. Elam, G.C. Schatz, M.J. Bedzyk, “Chemical-state specific atomic mapping of MoO_x catalyst on α -TiO₂(110) using X-ray standing wave excited XPS”, Bulletin of the American Physical Society, Virtual, March 2021, (Oral)
- Y. Chen, L. Jones, A. Das, T. L. Lee, D. T. Keane, G. C. Schatz, M. J. Bedzyk, “Site-specific valence-band of Pt monolayer on SrTiO₃ (001) via X-ray standing wave excited photoelectron emission”, Bulletin of the American Physical Society, Virtual, March 2021, (Oral)
- A. Das, “Chemical-state specific atomic mapping of VO_x/ α -TiO₂(110)”, 37th Annual Hilliard symposium, May 2020, Northwestern University (Nominated Talk)
- A. Das, Y. Chen, T. Lee, KVLV Narayanachari, M. Bedzyk, “3D atomic mapping of rutile-TiO₂ (110) supported Vanadium oxide catalyst using X-ray Standing Wave excited XPS”, Bulletin of the American Physical Society, Virtual, March 2020. (Oral)
- Y. Chen, A. Das, T. Lee, M. Bedzyk, “Structure and electronic states of Pt/SrTiO₃ (001) interface using X-ray standing wave excited photoelectron emission”, Bulletin of the American Physical Society, Virtual, March 2020 (Oral)

- **A. Das**, KVLV Narayanachari, B. H. Liu, D.T. Keane, M. J. Bedzyk, “*Oxidation state sensitive 3D atomic mapping of oxide-supported catalysts through X-ray Standing Wave (XSW) excited X-ray photoelectron spectroscopy (XPS)*”, Bulletin of the American Physical Society, Boston (USA), March 2019, (Oral)
- **A. Das**, B. H. Liu, D.T. Keane, J. Rix, M. J. Bedzyk, “*Integration of Hard X-ray Photoelectron Spectroscopy to X-ray Standing Wave Capability*”, The 15th International Surface X-ray and Neutron Scattering Conference, Pohang (South Korea), April 2018, (Poster)
- **A. Das**, B. H. Liu, D.T. Keane, J. Rix, M. J. Bedzyk, “*Addition of HAXPES to X-ray Standing Wave Capability at APS Sector 5*”, Hard X-ray Photoelectron Spectroscopy (HAXPES) Conference, Berkeley (USA), Sept. 2017, (Poster)
- **A. Das**, “*Surface structure-function relationship studies using hard X-ray photoelectron spectroscopy*”, Ipatieff Catalysis Symposium, Northwestern University (USA), Sept. 2017, (Poster)

EXPERTISE

Laboratory experience:

- Atomic Layer Deposition (ALD)
- Atomic Force Microscopy (AFM)
- X-ray photoelectron spectroscopy (XPS)
- X-ray absorption fine structure (XAFS)
- X-ray absorption near edge spectroscopy (XANES)
- Low-energy electron diffraction (LEED)
- Scanning tunnelling microscopy (STM)
- X-ray diffraction (XRD) and X-ray reflectivity (XRR)
- X-ray fluorescence spectroscopy (XRF)
- Scanning electron microscopy (SEM)
- Ultra-High Vacuum (UHV) chamber works
- Synchrotron source experiments

Software proficiency:

- MATLAB
- Mathematica
- CasaXPS
- CrystalMaker
- SingleCrystal
- IGOR
- Advantage

PROFESSIONAL AND TEACHING EXPERIENCE

- Organizer of “Leaders in energy and environment segment” at American Vacuum Society (AVS) symposium in October 2020
- REU Summer Research Program Mentor, May 2018 – July 2018
- Graduate Teaching Assistant
 - Course *MSE 361: Crystallography and Diffraction (Theory + Laboratory)* - (2018)
 - Course *MSE 461: Diffraction Methods in Material Science (Theory + Laboratory)* - (2018)

OUTREACH WORKS

- Member of the National Service Scheme at IIT Kharagpur (2012-2015)
 - Initiated Women Empowerment program to teach older women in remote Indian villages
 - Installed sewing machines in the village to encourage economic independence of the women
 - Yearly food and cloth collection and distribution in the village
- Awarded Medal of Appreciation from IIT Kharagpur for contribution to National Service Scheme.

OTHER ACTIVITIES

- Member of the Design and Fine Arts Team of IIT Kharagpur (2013-2014)
- Member of the Dramatics Society, IIT Kharagpur (2012-2013)
- Intermediate level chess player (online ELO rating 1100)
- Hobbies include painting, sketching, knitting and puzzle-solving