Curriculum Vitae

Jyoti Kuntail

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Jyoti Kuntail - Google Scholar

OBJECTIVE

Being a highly motivated researcher with good attitude, strong analytical and development skills, wanted to become part of Academic and fulfill my desire of acquiring the knowledge and pleasure in working with the most competent professionals and contribute to the growth of organization and simultaneously to create a personal satisfying career in the field of Research and Development.

ACADEMIC BACKGROUND

2016-2021	:	**Ph. D. (Physical Chemistry/Computational Chemistry)** Research supervisor: ***Dr. Indrajit Sinha***, Associate Professor, Department of Chemistry, Indian Institute of Technology-BHU, Varanasi. Thesis Title: **"Adsorption and Catalysis on magnetite, graphene oxide and their composites"** {Research Work carried out at (IIT BHU) India Varanasi, India (20^{th} June 2017 to 20^{th} Dec 2021), **Awarded date: 20^{th} Dec 2021**
2013-2014	:	**B.Ed.,** First division with **71.88%** from Rajasthan University, Jaipur, India.
2010 – 2012	:	**M.Sc.** (Physical Chemistry): First division with **70.54%** from Jamia Millia Islamia, Jamia Nagar, New Delhi, India. **Thesis Title**: "**LCAO approach to molecular wave functions of Hydrogen molecular ion".** Research supervisor: ***Dr. Sapan Kumar Jain***, Assistant Professor, Department of Chemistry, Jamia Millia Islamia, New Delhi.
2006 – 2009	:	**B.Sc.** (Hons.) Chemistry: First division with **60.74%** from Atma Ram Sanatan Dharma College, Delhi University, India.

LIST OF PUBLICATIONS

- **Kuntail, J.**, Verma, A., Kumar, S., & Sinha, I. (2021). Photo-Fenton interfacial phenomena on graphene oxide: computational and experimental investigations. *Journal of Molecular Liquids*, 117461. **(Ph.D. work)**
- **Kuntail, J.**, Pal, S., & Sinha, I. (2020). Interfacial phenomena during Fenton reaction on starch stabilized magnetite nanoparticles: Molecular dynamics and experimental investigations. *Journal of Molecular Liquids*, *318*, 114037. **(Ph.D. work)**
- **Kuntail, J.**, Jain, Y. M., Shukla, M., & Sinha, I. (2019). Adsorption mechanism of phenol, p-chlorophenol, and p-nitrophenol on magnetite surface: A molecular dynamics study. *Journal of Molecular Liquids*, *288*, 111053. **(Ph.D. work)**
- **Kuntail, J.**, Kumar, U., & Sinha, I. Insight into photo-Fenton reaction on a magnetite-GO nanocomposite: computational and experimental investigations. [First revision in Molecular Catalysis, March 2022]. **(Ph.D. work)**
- Kumar, U., **Kuntail, J.**, Kumar, A., Prakash, R., Pai M. R., & Sinha, I. (2022) In-situ H_2O_2 production for tetracycline degradation on Ag/s-(Co_3O_4/$NiFe_2O_4$) visible light magnetically recyclable photocatalyst. *Applied Surface Science, 589,* 153013.
- **Kuntail, J.***, Kavita*, Verma, D. K., Kumar, B., Singh, A. K., Shukla, N., Sinha, I., & Rastogi, R. B. (2020). Theoretical and experimental studies of pyranopyrazoles and their tribological compatibility with a borate ester. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, *606*, 125497. **(*Equal contribution, Collaboration work with other labs)**
- Verma, D. K*., **Kuntail, J.*,** Kumar, B., Singh, A. K., Shukla, N., Kavita, ... & Rastogi, R. B. (2020). Amino Borate-Functionalized Reduced Graphene Oxide Further Functionalized with Copper Phthalocyanine Nanotubes for Reducing Friction and Wear. *ACS Applied Nano Materials*, *3*(6), 5530-5541. **(*Equal contribution, Collaboration work with other labs)**
- Jatav, N., **Kuntail, J.,** Khan, D., De, A. K., & Sinha, I. (2021). AgI/CuWO4 Z-scheme photocatalyst for the degradation of organic pollutants: Experimental and molecular dynamics studies. *Journal of Colloid and Interface Science*, *599*, 717-729.
- Verma, A., Pal, S., **Kuntail, J**., Kamal, N., Mandal, R. K., & Sinha, I. (2021). Visible light enhanced p-nitrophenol reduction by glycerol over Ag/Cu core-shell bimetallic nanocatalysts. *Journal of Environmental Chemical Engineering*, *9*(4), 105655.
- Kumar, B., **Kuntail, J**., Verma, D. K., Rastogi, R. B., & Sinha, I. (2019). Mechanism of triboactivity of Schiff bases: Experimental and molecular dynamics simulations studies. *Journal of Molecular Liquids*, *289*, 111171. **(Collaboration work with other labs)**
- Jain, Y. M., **Kuntail, J**., Mukherjee, A., & Sinha, I. (2019). Computational Insight into the Mechanism of Arsenous Acid Adsorption on Magnetite (311) Surface.
- Kumar, S., Pal, S., **Kuntail, J**., Kumar De, A., & Sinha, I. (2019). Construction of a Visible Light Z-scheme Photocatalyst: Curcumin Functionalized Cu2O/Ag Nanocomposites. *ChemistrySelect*, *4*(36), 10709-10718.
- Kumar, S., Pal, S., **Kuntail, J**., & Sinha, I. (2019). Curcumin functionalized CuO/Ag nanocomposite: Efficient visible light Z-scheme photocatalyst for methyl orange degradation. *Environmental Nanotechnology, Monitoring & Management*, *12*, 100236.

NATIONAL/INTERNATIONAL CONFERENCE

- Attended 7th National Symposium on Solid State Chemistry & Allied Areas ISCAS 2011.
- **5th International Conference on Advanced Nanomaterials & Nanotechnology** IIT Guwahati, Adsorption isotherms of Phenol, p-chlorophenol and p-nitrophenol on Magnetite 001 Plane: Molecular Dynamics Simulation 2017 **Poster presentation**.
- International Conference on Advanced Materials, Energy & Environmental Sustainability (**ICAMEES**) UPES Dehradun, Simulation of adsorption behaviour of phenol, p-chlorophenol and p-nitrophenol on (111) Magnetite surface 2018 **Oral Presentation**.

- **Symposium on Molecular Simulation of Complex Fluids and Interfaces 2020** IIT Kanpur, Understanding the Adsorption Mechanism of Arsenous Acid on Magnetite (311) Surface through Molecular Dynamics Simulations 2020 **Poster presentation**.
- 1st international Online Conference on Blends, Composites, Bio-Composites and Nanocomposites **(ICNC)** Kerala India, Adsorption mechanism on starch stabilized magnetite nanoparticles 2020 **Paper presentation**.
- **Virtual Winter School on Computational Chemistry,** Interfacial phenomena during Fenton reaction on starch stabilized magnetite nanoparticles: molecular dynamics and experimental investigations 2021 **Single Figure Presentation (SFP)**
- International Conference on Advanced Materials for better Tomorrow (AMBT-2021), IIT BHU, Varanasi, 13 - 17th July 2021**, Flash talk (Poster Presentation)**.
- **Virtual Winter School on Computational Chemistry,** Insight into photo-Fenton reaction on a magnetite-GO nanocomposite: computational and experimental investigations. 2022 **Single Figure Presentation (SFP)**

WORKSHOP

- National Workshop on **Challenges and Opportunities in Chemistry**, Maitreyi College, University of Delhi,22-23th September 2006.
- One-day seminar on **Chemistry in our lives-Issues and Challenges JMI, New Delhi**, Nanochemistry in Daily life **2011 Poster Presentation.**
- Five-day workshop on **Introduction to Gaussian: Theory and Practice** held by Scube Scientific Software solutions in Delhi,2018.
- A workshop on **Fundamental of Molecular Simulations,** IIT Kanpur, 17 - 21th February 2020.
- A workshop on **Molecular modeling of materials and biological macromolecules Simulations,** NIT Rourkela, 22-26th September 2020.
- NSM online workshop on **HPC workshop**, IIT Dharwad and IIT Palakkad, 20-27th March 2021.
- NSM online workshop on **Simulation Methods in Scientific Computing**, Indian Institute of Technology Kharagpur, 14-16th June 2021.

SKILLS

PROGRAMMING LANGUAGE: Python, Qbasic
ENVIRONMENT: Window/Linux
SOFTWARES: LAMMPS, Gaussian, Quantum Espresso, VMD, MAPS(Scienomics), Avogadro, Packmol, Origin, MS office.
PROFESSIONAL TRAINING: Uv-Visible spectrophotometer, FT-IR, XRD
LANGUAGE SKILL: Proficiency in English, Hindi (Native)

SCHOLASTIC ACHIEVEMENTS

- Got **MHRD Fellowship** from Govt. of INDIA at **IIT-BHU** during December 2016 to December 2021.
- **Qualified** Graduate Aptitude Test in Engineering (**GATE-2016**) from Chemistry with an AIR -1438
- **First rank** in **Poster Presentation** at one-day seminar on "Chemistry in our lives-Issues and Challenges", organized by JMI on March 28, 2011, New Delhi.
- **First rank** in Research Presentation at **National Event on "4 Minute Research Pitch**" organized by Department of Chemistry of IIS (deemed to be University), Jaipur in collaboration with Govt. Madhav Science PG College, Ujjain on 15-16th April 2022.

TEACHING ASSITANTSHIPS

- Tutor of Chemistry-101 (CY-101) course in IIT BHU (July 2018-November2018), (July 2019-November2019). [B. Tech 1st semester]
- Experimental Lab tutor of Chemistry-101 (CY-101) course in IIT BHU (July 2017-November2017), (July 2018-November2018). [B. Tech 1st semester]
- Experimental Lab tutor of Physical chemistry-DP-CY-494) course in IIT BHU (Jan 2020-March2020), (Feb2021-April2021) M.Sc. 2nd semester) [Designed Gaussian experiments and conducted Lab, Assistant to Dr. Indrajit Sinha].

EXTRA CURRICULAR ACTIVITIES

- Active participant of Chemistry Subject Association during undergraduate, Postgraduate level and PhD level.
- Participated in Quiz competition and social activity.
- N.C.C Cadet for 3 yrs. in 3 DELHI GIRLS BN N.C.C (NATIONAL CADET CORPS) 'C' Certificate holder.

PERSONAL BIODATA

Date of Birth	08th November, 1988
Nationality	Indian
Marital Status	Unmarried

ACADEMIC REFERENCES

Dr. Indrajit Sinha (Associate Professor) Department of Chemistry, IIT-BHU Varanasi, India Contact: +919235846141 Email: isinha.apc@iitbhu.ac.in	Dr. (Mrs.) R.B. Rastogi (Retired Professor), Department of Chemistry, IIT-BHU Varanasi, India. Contact: +919953602564 Email: rashmi.apc@iitbhu.ac.in