# Curriculum Vitae

***Dr. Manzoor Ahmad Dar***
***Assistant Professor,***
***Department of Chemistry,***
***Islamic University of Science and Technology,***
***Awantipora, India***

## Personal Information

*Date of Birth: 01-04-1985 Citizenship: Indian.*
*Marital Status: Single*
*Current Address: Department of Chemistry, Islamic University of Science and Technology, Awantipora, India.*
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## Research Interests

The primary focus of my research encompasses the theoretical understanding of structure, electronic and catalytic properties of nanoclusters, transition metal complexes, and surfaces for small molecule activation and energy applications. I am extremely interested in working on challenging problems based on energy conversion processes such as **Oxygen Reduction Reaction, Nitrogen Reduction, and $CO_2$ Reduction Reaction** using homogeneous and heterogeneous catalysts. Moreover, I am highly interested in investigating the structure and dynamics of proteins and drug molecules, and their interaction with metal nanoclusters.

## Projects and Research grants

1. Start-up Research grant on "*Development of theoretical descriptors for the rational design of single-atom catalysts for $CO_2$ hydrogenation using first principle simulations*". (**SERB-DST Govt. of India) Rs. 24.20 lakhs**
2. Start-up grant on *"Computational insights into the design of size-selected cage-type and core-shell nanoclusters with low platinum loading for oxygen reduction reaction".* **(UGC Govt. of India) Rs. 10 lakhs**

## Publications after joining IUST

1. Anjumun Rasool Ganie, Insha Anis Bhat, Mudit Dixit, Ashakiran Maibam, Afshana Hassan Dar, Sailaja Krishnamurty and **Manzoor Ahmad Dar***. Tantalum based single, double and triple atom catalysts supported on g-$C_2N$ monolayer for effective nitrogen reduction reaction: A comparative DFT investigation. *Catal. Sci. Technol.*, **2021**, (https://doi.org/10.1039/D1CY01292D)

   ***RSC (Impact Factor=6.119)***
2. Ashakiran Maibam, Sailaja Krishnamurty and **Manzoor Ahmad Dar*.** Electrocatalytic nitrogen reduction directed through the p-band center of boron on $B_{SAC}$@$Mo_2C$. *Mater. Adv.*, **2021**, (https://doi.org/10.1039/D1MA00953B)

   ***RSC (Impact Factor=NA)***
3. Krati Joshi, Sailaja Krishnamurty and **Manzoor Ahmad Dar*.** Surface functionalization: an efficient alternative for promoting the catalytic activity of closed shell gold clusters. *Phys. Chem. Chem. Phys.* **2020**, *22*, 23351-23359

   ***RSC (Impact Factor=3.676)***
4. Sailaja Krishnamurty and **Manzoor Ahmad Dar***. Molecular and Dissociative Adsorption of Oxygen on Au–Pd Bimetallic Clusters: Role of Composition and Spin State of the Cluster.

*ACS Omega*, **2019**, *4*, 12687−12695.

***ACS (Impact Factor=3.512)***

## Publications before joining IUST

5. **Dar Manzoor*,** Sailaja Krishnamurty and Sourav Pal*. Contriving a Catalytically Active Structure from an Inert Conformation: A Density Functional Investigation of Al, Hf, and Ge Doping of $Au_{20}$ Tetrahedral Clusters. *J. Phys. Chem. C*, **2016**, *120*, 19636–19641.

   ***ACS (Impact Factor=4.126)***

6. **Dar Manzoor*,** Sailaja Krishnamurty and Sourav Pal*. Endohedrelly Doped Gold Cages: Efficient Catalysts for Oxygen Activation and CO Oxidation. *Phys. Chem. Chem. Phys.* **2016**, *18*, 7068-7074.

   ***RSC (Impact Factor=3.676)***

7. **Dar Manzoor*** and Sourav Pal*. Reactivity and Catalytic Activity of Hydrogen Atom Chemisorbed Silver Clusters. *J. Phys. Chem. A* **2015**, *119*, 6162−6170.

   ***ACS (Impact Factor=2.781)***

8. **Dar Manzoor** and Sourav Pal*. Hydrogen Atom Chemisorbed Gold Clusters as Highly Active Catalysts for Oxygen Activation and CO Oxidation. *J. Phys. Chem. C* **2014**, *118*, 30057−30062.

   ***ACS (Impact Factor=4.126)***

9. **Dar Manzoor**, Sailaja Krishnamurty and Sourav Pal*. Effect of Silicon Doping on the Reactivity and Catalytic Activity of Gold Clusters. J. *Phys. Chem. C* **2014,** *118*, 7501−7507.

   ***ACS (Impact Factor=4.126)***

10. Achintya K. Dutta, **Dar Manzoor**, Nayana Vaval and Sourav Pal*. Structure, Stability, and Properties of the Trans Peroxo Nitrate Radical: The Importance of Nondynamic Correlation. *J. Phys. Chem. A* **2014**, *118*, 1350−1362.

    ***ACS (Impact Factor=2.781)***

11. **Dar Manzoor**, Sourav Pal* and Sailaja Krishnamurty*. Influence of Charge and Ligand on the Finite Temperature Behavior of Gold Clusters: A BOMD Study on $Au_6$ Cluster. *J. Phys. Chem. C* **2013**, *117*, 20982−20990.

    ***ACS (Impact Factor=4.126)***

12. **Dar Manzoor** and Sourav Pal*. Enhanced interaction of molecular oxygen with amino acid complexes of silver and gold clusters. *Indian Journal of Chemistry* **2014,** *53A*, 996-1000.

    ***(Impact Factor=0.494)***

## Education and Degrees

1. **Project post-doctoral fellow with Prof. Vardharajan Srinivasan** at Department of Chemistry, **Indian Institute of Science Education and Research**, Bauri Bhopal, India ***(*Project Title: *Methane Activation on Single Iron Atom Catalysts Impregnated in Silica Matrix)***
2. **Doctor of philosophy** in Quantum Chemistry and Computational Material Sciences with **Prof. Sourav Pal** from **CSIR-National Chemical Laboratory, India.**

   Thesis Title: Ab-initio Molecular Dynamics and Density Functional Based Studies on the Stability, Reactivity and Catalytic Properties of Silver and Gold Clusters (January 2011 to February 2016 ).
3. **Master of Science** (***Physical Chemistry***) **with I$^{st}$ division** from Department of Chemistry, University of Kashmir, Jammu and Kashmir, India in year (*2008 to 2010*).
4. **July 2005- July 2008: Bachelor of Science** with I$^{st}$ division from University of Kashmir, Jammu and Kashmir, India.

## Offers and Fellowships

1. Offered **Scientist I** position at **Institute of High Performance Computing**, A*STAR, Singapore (December 2015).
2. Offered Postdoctoral Research Associate position by **Prof. Mu-Hyun Baik** at the Institute of Basic Sciences, **Korea Advanced Institute of Science and Technology** (KAIST), Daejeon, Korea (February 2017).
3. Qualified **CSIR-UGC National Eligibility Test for Lectureship** (December 2009)
4. Qualified **CSIR-UGC National Eligibility Test for Junior Research Fellowship** (June 2010).
5. M. Sc Entrance topper, Department of Chemistry, (1 year fellowship) University of Kashmir (2008 Batch)

## Computational Skills

1. I am quite confident in handling many DFT and /or TDDFT based packages to study the electronic, catalytic and optical properties of nanomaterials. Packages which I have to publish (am using currently) some of my works include **Gaussian09, deMon2K, NwChem, Quantum Espresso, CP2K and VASP.**
2. I have also good experience in Born-Oppenheimer molecular dynamics simulations (BOMD) to study the finite temperature behavior of materials. I have used codes such as **CPMD, deMon2k and VASP for BOMD simulations**.
3. I have also working experience with **Material Studio** and global optimization codes such as **GMIN, CALYPSO, etc.** for finding the lowest energy structures of nanoclusters.
4. I have written codes in FORTRAN language to find the root mean square and mean square deviations along the trajectories generated during BOMD simulations. Moreover, I was also involved with my group members to understand the basic formulation of the coding in Hatree-Fock method.
5. I also administered ESTG group clusters for 2 years and have installed codes such as VASP, Quantum Espresso, CPMD, etc in both serial and parallel modes on work-stations and clusters.
6. I am also very well aware and used to graphical user interfaces such as ***Molden, Xcrysden, VESTA, P4v, Avogadro, GaussView, VMD, Chemcraft, Chemdraw, GNUPlot, Microsoft Pwerpoint, Latex, Microsoft word, office, Adobe Illustrator***.

## Teaching Interests

1. Basic and Advanced Quantum Mechanics
2. Electrochemistry and Solid-state Chemistry
3. Chemical Thermodynamics
4. Chemical Kinetics
5. Molecular Spectroscopy

## Invited talks/Conferences organized/attended/Posters presented

1. Delivered an invited talk on "*Structural Modulation of Gold Clusters for Enhanced Catalytic Activity: Insights from Density Functional Theory*" in the international conference on Structure and Dynamics of Molecular and Condensed Matter Systems, ICSD – 2020 organized by IISER, Kolkata.
2. Delivered an online talk on "*Density Functional Theory as a Tool to Simulate the Reactivity and Catalytic Properties of Materials*" at the Interdisciplinary Division for Renewable

Energy and Advanced Materials, NIT Srinagar.

3. Participated in one week "*Summer School on Quantum Mechanics*" organized by Department of Physics, IUST Awantipora in 2019.
4. Participated in One Week Faculty Development Program on Emerging Trends in Physical, Chemical and Mathematical Sciences organized by Departments of Physics, Chemistry and Mathematical Sciences, IUST Awantipora.
5. Participated and presented a poster in a Symposium organized at Department of Chemistry, Indian Institute of Science Education and Research, Bhopal-2016.
6. Participated and presented a poster in "Frontiers in Electronic Structure Theory 2015" (FEST- 2015), Goa.
7. Presented poster during the Science Day celebrations at CSIR- National Chemical Laboratory, Pune-2015.
8. Participated and presented a poster in "Theoretical Chemistry Symposium 2014" (TCS-2014), CSIR-National Chemical Laboratory, Pune and Indian Institute of Science Education and Research, Pune.
9. Participated and presented a poster in a Symposium organized during the National Science Day celebrations at CSIR- National Chemical Laboratory, Pune-2014.

## Additional positions held at IUST, Awantipora

1. Nodal Officer, (Department of Chemistry) DIQA, IUST (Since 2018 –till date).
2. Nodal Officer. Centre for Vocational Studies (June 2019 – till date)

## References and Probable Collaborators

### 1. Prof. Sourav Pal (Research Supervisor)

Director, IISER Kolkata & Former Director,
CSIR-National Chemical Laboratory, Pune, India.
Email: s.pal@iiserkol.ac.in ; s.pal@ncl.res.in

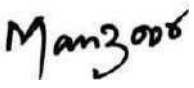
### 2. Dr. Sailaja Krishanamurthy

Scientist,
Physical and Material Chemistry Division,
CSIR- NCL, Pune
Email: sailaja.raaj@gmail.com

### 3. Prof. Achintya K. Dutta

Department of Chemistry,
Indian Institute of Technology Bombay.
Email: achintya@chem.iitb.ac.in

I certify that to the best of my knowledge and belief this resume correctly describes my qualifications and me.



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