

# Mudit Dixit

*Senior Scientist, CSIR-CLRI*

## Academic Qualifications

- 2008–2015 **Doctor of Philosophy (Ph.D.)**, *Theoretical and Computational Chemistry, India.*  
National Chemical Laboratory (a premier institute of Council of Scientific and Industrial Research (CSIR), under the supervision of Prof. Sourav Pal.
- 2006–2008 **Master of Science (Chemical Sciences)**, *India.*  
Pondicherry Central University, Pondicherry.
- 2003–2006 **Bachelor of Science (Chemistry, Physics, and Mathematics)**, *India.*  
S.S. College (Rohilkhand University), Shahjahanpur

## Research Experience

- 2017–2019 **Postdoctoral Researcher**, *University of Pittsburgh, Pittsburgh, USA.*  
Dehydrogenation of alkanes on metals oxides,  $CO_2$  reduction on metal carbides, and design of new catalysts for methane activation.  
**Supervisor** – Prof. Giannis Mpourmpakis
- 2014–2016 **Postdoctoral "PBC" Research Fellow**, *Bar-Ilan University, Ramat Gan, Israel.*  
Design and investigation of cathode materials for Li-ion batteries, and Enzyme Catalysis using ab-initio (First principles), DFT and Molecular Dynamics simulations.  
**Supervisor** – Prof. Dan Thomas Major
- 2010–2013 **Senior Research Fellow (Ph.D.)**, *CSIR-National Chemical Laboratory, Pune, India.*  
*Ab-initio*, DFT and Molecular Dynamics investigations of hydrogen storage materials.  
**Supervisor** – Prof. Sourav Pal
- 2008–2010 **Junior Research Fellow at National Chemical Lab)**, *CSIR-National Chemical Laboratory, Pune, India.*  
*Ab-initio* investigations of hydrogen storage materials.  
**Supervisor** – Prof. Sourav Pal
- 2006–2008 **M. Sc. Dissertation**, *Pondicherry Central University, Pondicherry, India.*  
Computational study of ring-currents in aromatic molecules.  
**Supervisor** – Prof. M.M. Balakrishna Rajan

## Teaching experience

- Jan 2022–Feb 2023 **Assistant Professor**, *BITS, Pilani, Hyderabad Campus, Hyderabad, India.*

## Present Academic Appointment

- March 2023– **Senior Scientist**, *CSIR-CLRI, Chennai, India.*

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## Awards and Fellowships

- 2014 **Planning and Budgeting Committee (PBC) Postdoctoral fellowship, Israel.**  
A fellowship program for outstanding postdoctoral researchers
- 2008 **Qualified Graduate Aptitude Test in Engineering (GATE), India.**  
Conducted by the Indian Institute of Technology (IIT)
- 2008 **Junior Research Fellowship (JRF), India.**  
Awarded by Council of Scientific and Industrial Research (CSIR), India, a premier national R&D organization
- 2008 **Qualified National Eligibility Test (NET), India.**  
Conducted by CSIR and University Grant Commission (UGC)

## Area of Interest

- Electrochemical Energy Storage using First principles-based methods
- Computational Heterogeneous Catalysis
- Enzyme Catalysis using Multi-scale methods

## Publications, h-index=25, Total citations=3700+

55. Singh, P.; Adithya K.R. **Dixit, M.\***. Unraveling the Contribution of Cationic and Anionic Redox in Na-rich Cathode Materials through First-Principles Calculations *ACS applied Electronic Materials* **2024** just accepted (IF=4.3)
54. Gogoi, A.; **Dixit, M.\***, Sourav Pal\*. Mechanistic Insight of High-Valent First-Row Transition Metal Complexes for Dehydrogenation of Ammonia Borane *J. Phys. Chem. A* **2024** just accepted DOI: <https://doi.org/10.1021/acs.jpca.4c04069> (IF=2.7)
53. Borah, R.K.; Singh, P.; **Dixit, M.**, Vernekar, A.A. A Ru atomic cluster-installed Co–Co<sub>2</sub>B nanocatalyst remarkably combats product inhibition while sustaining high turnover frequency of hydrogen production *J. Mater. Chem. A* **2024**, 12, 20256–20269.(IF=10.7)
52. Singh, P. **Dixit, M.\*** Stabilizing Anionic Redox and Tuning Its Extent in Na-Rich Cathode Materials through Electronic Structure Engineering *J. Phys. Chem C* **2024**, 128, 8883–8893.(IF=3.3)
51. Anamika Bandyopadhyay, Adarash Kumar Shukla, Priti Singh, Ashutosh Mahale, Shivkumar Sharma Irukuvajjula, Ramakrishna Vadrevu, Onkar P Kulkarni, **Mudit Dixit**, Anupam Bhattacharya, Nickel-assisted selective detection of histidine and histidine-rich proteins via an ON-OFF-ON fluorescent probe and its imaging in live cells *Journal of Photochemistry and Photobiology A: Chemistry* **2023**, 443, 114885.(IF=4.1)
50. Gupta, N. Halder, S. Behere, R.P., Singh, P. Kanungo, S. **Dixit, M.\***, Chanchal Chakraborty\*, and Biplab Kumar Kuila\* Side-Chain Modification in Conjugated Polymer Frameworks for the Electrocatalytic Oxygen Evolution Reaction *ACS Appl. Mater. Interfaces* **2023**, 15, 24, 29042–29051.(IF=9.5)
49. Fozia, S.; Hassan, A.; Reshi, S. A.; Singh, P.; Bhat, G. A.; **Dixit, M.\***; Dar, M.A.\* Boosting

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CO<sub>2</sub> Activation and Reduction by Engineering the Electronic Structure of Graphitic Carbon Nitride through Transition Metal-Free Single-Atom Functionalization *J. Phys. Chem. C* 2023 (just accepted)(**IF=4.1**)

**48.** Singh, P.; Gogoi, A.; Aien, Q. U.; **Dixit, M.\***, Assessing the Effect of Dopants on the C H Activation Activity of -Al<sub>2</sub>O<sub>3</sub> using First-Principles Calculations. *ChemPhysChem* **2023**, 24 (5), e202200670.(**IF=3.5**)

**47.** Leelasree, T.; **Dixit, M.**; Aggarwal, H., Cobalt-Based Metal–Organic Frameworks and Its Mixed-Matrix Membranes for Discriminative Sensing of Amines and On-Site Detection of Ammonia. *Chemistry of Materials Chem. Mater.* **2023**, 35, 2, 416–423.(**IF=10.5**)

**46.** Singh, P.; **Dixit, M.\***, Opportunities and Challenges in the Development of Layered Positive Electrode Materials for High-Energy Sodium-Ion Batteries: A Computational Perspective. *Langmuir* **2023**, 39, 1, 28–36(**IF=4.33**)

**45.** Halder, S.; Roy, S.; **Dixit, M.**, Chakraborty, C.A terpyridine based hydrogel system for reversible transmissive-to-dark electrochromism and bright-to-quenched electrofluorochromism. *Chem. Commun.* **2022**, 2022, 58 (60), 8368-8371.(**IF=4.6**)

**44.** Rasool, A.; Anis, I.; **Dixit, M.**; Maibam, A.; Hassan, A.; Krishnamurthy, S.; Dar, M. A., Tantalum based single, double, and triple atom catalysts supported on gC 2 N monolayer for effective nitrogen reduction reaction: a comparative DFT investigation. *Catalysis Science Technology* **2022**, 12 (1), 310-319).( **IF=6.1**)

**43.** Penjarla, T. R.; Shukla, A. K.; Hazra, R.; Roy, D.; Kundarapu, M.; **Dixit, M.**; Bhattacharya, A., Copper acetate catalysed C–C bond formation en route to the synthesis of spiro indanedione cyclopropylpyrazolones. *Organic Biomolecular Chemistry* **2022**, 20 (18), 3779-3784.(**IF=3.89**)

**42.** Mukherjee, N.; Satyanarayana, A. N.; Singh, P.; **Dixit, M.**; Chatterjee, T., Recyclable iodine-catalyzed radical selenylative annulation of 2-alkynyl biaryls with diselenides in water: a green approach to selenyl polycyclic aromatic hydrocarbons and polycyclic heteroaromatics. *Green Chemistry* **2022**, 24 (18), 7029-7038.(**IF=9.8**)

**41.** Gogoi, A.; Singh, P.; Pal, S.\*; **Dixit, M.\***, Unraveling the Mechanistic Details of Ru–Bis (pyridyl) borate Complex Catalyst for the Dehydrogenation of Ammonia Borane. *Inorganic Chemistry* **2022**, 61 (27), 10283-10293.(**IF=5.4**)

**39.** Li,W.; Taylor, M.G.; Bayerl,D; Mozaffari,S; **Dixit, M** et al. Solvent manipulation of the pre-reduction metal–ligand complex and particle-ligand binding for controlled synthesis of Pd nanoparticles. *Nanoscale*, **2021**, 13, 206-217(**IF=7.79**)

**38.** Juneau, M.; Vonglis, M.; Hartvigsen, J.; Frost, L.; Bayerl, D.; **Dixit, M.**; Mpourmpakis, G.; Morse, J. R.; Baldwin, J. W.; Willauer, H.; Porosoff, M. D.; Assessing the viability of  $K - Mo_2C$  for reverse water-gas shift scale-up: Molecular to laboratory to pilot scale. *Energy Environ. Sci.*, **2020**,13, 2524-2539 (**IF=39.6**)

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37. Chakraborty, A.; Kunnikuru, S.; Kumar, S.; Markovsky, B.; Aurbach, D.; **Dixit, M.**; Major, D. T.; Layered Cathode Materials for Lithium-Ion Batteries: Review of Computational Studies on  $LiNi_{1-x-y}Co_xMn_yO_2$  and  $LiNi_{1-x-y}Co_xAl_yO_2$ . *Chem. Mater.* **2020** 32 (3), 915-952 (IF=10.15)
36. Chakraborty, A.; Kunnikuru, S.; **Dixit, M.**; Major, D. T.; Review of Computational Studies of NCM Cathode Materials for Li-ion Batteries. *In press Isr. J.* **2020**, 60 (8-9), 850-862, (IF=3.33)
35. Mozaffari, S; Li, W; **Dixit, M.**; Seifert, S.; Lee, B.; Kovarik, L.; Mpourmpakis, G.; Karim, A. M.; The Role of Nanoparticle Size and Ligand Coverage in Size Focusing of Colloidal Metal Nanoparticles *Nanoscale Adv.*, **2019**, 1, 4052-4066 (IF=4.55)
34. Kaiyang, T; **Dixit, M**; Daeon, J.; Mpourmpakis, G. Predicting Metal-Support Interactions in Oxide-Supported Single-Atom Catalysts *Ind. Eng. Chem. Res.* **2019**, 58, 44, 20236-20246 (IF=3.37)
33. **Dixit, M**; Cholewinski, M; Mpourmpakis, G. Computational Study of Methane Activation on  $\gamma - Al_2O_3$  *ACS Omega* **2018**, 3, 12, 18242-18250. (IF=2.87)
32. Kostetsky, P; Carly, N; **Dixit, M**; Mpourmpakis, G. Understanding Alkane Dehydrogenation through Alcohol Dehydration on  $\gamma - Al_2O_3$  (*Ind. Eng. Chem. Res.* **2018**, 57, 49, 16657-16663). (IF=3.37)
31. **Dixit, M**; Kostetsky, P; Mpourmpakis, G. Structure-Activity Relationships in Alkane Dehydrogenation on  $\gamma - Al_2O_3$ : Site-Dependent Reactions (*ACS Catal.* **2018**, 8, 12, 11570-11578). (IF=12.35) (Featured on the front journal cover)
30. Estes, J.; **Dixit, M.**; Mpourmpakis, G. Understanding the Gas Phase Chemistry of Alkanes with First Principles Calculations, *J. Chem. Eng. Data*, **2018**, 63, 2430-2437. (IF=2.36)
29. Chakraborty, A.; **Dixit, M.**; Major, D.T., Predicting the Properties of Cathodes for Lithium-ion Batteries via the Strongly Constrained and Appropriately Normed density functional method *npj Computational Materials* - (Nature Publishing), 4, **2018** .(IF=9.34)
28. Weinreb, O; Singh, V; **Dixit, M**; Shmuel T.G.; Pitor, J; Fonseca, B; Major, D.T.; Fisher, B. M A Promising Drug Candidate for the Treatment of Glaucoma Based on a P2Y6-Receptor Agonist. *Purinergic Signaling*, **2018**, 14,3, 271-284. (IF=3.88)
27. Jun, D. W.; Kim, U. H.; Park, K. J.; Aurbach, D.; Major, D. T.; Goobes, G.; **Dixit, M.**; Leifer, N.; Wang, C.; Yan, P.; Ahn, D.; Kim, K. H.; Yoon, C. S.; Sun, Y. Y. Pushing the Limit of Layered Transition Metal Oxide Cathodes for High-Energy Density Rechargeable Li-ion Batteries. *Energy Environ. Sci.*, **2018**, 11, 1271-1279. (IF=33.32)
26. **Dixit, M.**; Weitman, M.; Gao, G; Major D.T. Comment on "Substrate Folding Modes in

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Trichodiene Synthase: A Determinant of Chemo- and Stereoselectivity" *ACS Catal.*, **2018**, 8, 1371–1375.(IF=12.35)

**25.** Kallitsakis, M.G; **Dixit, M**; Tancini, P.D.; Mpourmpakis, M.; Lykakis I. N. Mechanistic Studies on the Michael Addition of Amines and Hydrazines to Nitrostyrenes: Nitroalkane Elimination via a Retro-aza- Henry Type Process. *J. Org. Chem.*, **2018**, 83, 1176-1184. (IF=4.33)

**24.** **Dixit, M**; Markovsky, B; Schipper, F; Aurbach, D; Major D.T. The Origin of Structural Degradation during Cycling and Low Thermal Stability of Ni-Rich Layered Transition Metal- Based Electrode Materials *J. Phys. Chem. C*, **2017**, 121 (41), 22628–22636.(IF=4.18)

**23.** Schipper, F.; Bouzaglo, F.; **Dixit M.**; et al. From Surface  $ZrO_2$  Coating to Bulk Zr Doping by High Temperature Annealing of Nickel-Rich Lithiated Oxides and Their Enhanced Electrochemical Performance in Lithium Ion Batteries. *Adv. Energy Mater.* **2017**, 1701682. (IF=24.88)

**22.** **Dixit, M.**; Peng, X.; Porosoff, M. D.; Willauer, H.D.; Mpourmpakis, G.; Elucidating the role of oxygen coverage in  $CO_2$  reduction on  $Mo_2C$ . *Catal. Sci. Technol.*, **2017**, 7, 5521 (IF=5.72) (Featured on the front cover, selected as a hot article of 2017).

**21.** Schipper, F; Nayak, P.K. Erickson, E.M; Amalraj, S. F; Lavi, O. S; Rao, P.T; Talianker, M; Grinblat, J; Sclar, H; Breuer, O; Julien, C.M; Munichandraiah, NKovacheva, D; **Dixit, M**; Major, D.T; Markovsky, B; Aurbach, D. Study of Cathode Materials for Lithium-Ion Batteries: Recent Progress and New Challenges. *Inorganics* **2017**, 5(2), 32.

**20.** **Dixit, M**; Markovsky, B; Aurbach, D; Major, D.T. Unraveling the Effects of Al Doping on the Electrochemical Properties of  $LiNi_{0.5}Co_{0.2}Mn_{0.3}O_2$  Using First Principles. *J. Electrochem. Soc.*, **2017**, 164 (1) A6359-A6365 (IF=3.12) (Selected by the editor and featured on the front cover).

**19.** **Dixit, M**; Weitman, M; Gao, J; Major, D.T. Chemical Control in the Battle against Fidelity in Promiscuous Natural Product Biosynthesis: The Case of Trichodiene Synthase. *ACS Catal.*, **2017**, 7, 812–818. (IF=12.35)

**18.** Llave, E. D. L; Talaie, Elahe; Levi, Elena; Nayak, P. K. **Dixit, M**; Rao, P.T; Hartmann, P; Chesneau, F; Major, D. T. Greenstein, M; Aurbach, D; Nazar L. F. Improving Energy Density and Structural Stability of Manganese Oxide Cathodes for Na-Ion Batteries by Structural Lithium Substitution. *Chem. Mater.*, **2016**, 28, 9064–9076. (IF=9.56)

**17.** **Dixit, M.**; Schipper, F.; Kovacheva, D.; Talianker, M.; Haik,O.; Grinblat,Y.; Erickson, E.M.; Ghanty, C.; Dan T. Major, D.T.; Markovsky, B.; Aurbach, D. Stabilizing Nickel-Rich Layered Cathode Materials by a High-Charge Cation Doping Strategy: Zirconium-Doped  $LiNi_{0.6}Co_{0.2}Mn_{0.2}O_2$ . *J. Mater. Chem. A*, **2016**, 4,16073-16084 (IF=11.31)

**16.** Das, S.; **Dixit, M.**; Major, D. T. First Principles Model Calculations of the Biosynthetic Pathway in Selinadiene Synthase. *Bioorg. Med. Chem.* **2016**, 24, 4867-4870. (IF=3.07)

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**15. Dixit, M.;** Das, S.; Mhashal, A. R.; Eitan, R.; Major, D. T. Practical aspects of multiscale classical and quantum simulations of enzyme reactions. *Methods in Enzymology* **2016** (Invited review) 577, 251-286. (IF=2.00)

**14. Hevroni, B.L.;** Major, D.T.; **Dixit, M.;** Mhashal, A. R.; Das, S.; Fischer, B.; Nucleoside-2',3'/3',5'-Bis(thio)phosphate are Zn(II)/Cu(II)-Chelators Capable of Disassembly of Amyloid Beta(1-42)-Zn(II)/Cu(II) Aggregate. *Org. Biomol. Chem.* **2016**, 14, 4640- 4653. (IF=3.49)

**13. Dixit, M.;** Kosa, M.; Lavi, O.S.; Makrobosky, B; Aurbach, D.; Major, D. T. Thermodynamic and kinetic studies of  $LiNi_{0.5}Co_{0.2}Mn_{0.3}O_2$  as a positive electrode material for Li-ion batteries using first principles. *Phys. Chem. Chem. Phys.* **2016**, 18 (9), 6799-6812 (IF=3.43) Included in a themed collection "2016 most accessed PCCP articles".

**12. Singh, V.;** **Dixit, M.;** Kosa, M.; Major, D.T.; Levi E.; Aurbach, D.; Is it True that the Normal Valence-Length Correlation is Irrelevant for Metal-Metal Bonds? *Chem. Eur. J.* **2016**, 22,5269–5276. (IF=4.87)

**11. Dixit, M.;** Major, D. T.; Pal, S. Hydrogen adsorption in ZIF-7: A DFT and *ab-initio* molecular dynamics study. *Chem. Phys. Lett.* **2016**, 651,178–182. (IF=2.02)

**10. Azran, S.;** Danino, O.; Förster, D.; Kenigsberg, S.; Reiser, G.; **Dixit, M.;** Singh, V.; Major, D. T.; Fischer, B., Identification of Highly Promising Anti-Oxidants/ Neuroprotectants Based on Nucleoside 5'-Phosphorothioate Scaffold. Synthesis, Activity, and Mechanisms of Action *J. Med. Chem.* **2016**, 58 (21), 8427-8443. (IF=6.20)

**09. Dixit, M.;** Engel, H.; Eitan, R.; Aurbach, D.; Levi, M. D.; Kosa, M.; Major, D. T., Classical and Quantum Modeling of Li and Na Diffusion in  $FePO_4$ . *J. Phys. Chem. C* **2015**, 119, 15801-15809. (IF=4.18)

**08. Singh, V.;** Gershinsky, Y.; Kosa, M.; **Dixit, M.;** Zitoun, D.; Major, D. T., Magnetism in Olivine-Type  $LiCo_{1-x}Fe_xPO_4$  Cathode Materials: Bridging Theory and Experiment *Phys. Chem. Chem. Phys.* **2015**, 17 (46), 31202-31215.(IF=3.43)

**07. Aurbach, D;** Srur-Lavi, O; Ghanty, C; Dixit, M., et al., Studies of Aluminum- Doped  $LiNi_{0.5}Co_{0.2}Mn_{0.3}O_2$ : Electrochemical Behavior, Aging, Structural Transformations, and Thermal Characteristics. *J. Electrochem. Soc.* **2015**, 162, A1014-A1027. (IF=3.12)

**06. Sharma, V.;** **Dixit, M.;** Satsangi, V. R.; Dass, S.; Pal, S.; Shrivastav, R., Photoelectrochemical Splitting of Water with Nanocrystalline  $Zn_{1-x}Mn_xO$  Thin Films: First-Principle DFT Computations Supporting the Systematic Experimental Endeavor. *Int. J. Hydrogen Energy* **2014**, 39, 3637-3648. (IF=4.93)

**05. Kumar, K.;** **Dixit, M.;** Khire, J.; Pal, S., Atomistic Details of Effect of Disulfide Bond Reduction on Active Site of Phytase B from *Aspergillus Niger*: A Md Study. *Bioinformation* **2013**, 9, 963.

**04. Dixit, M.;** Adit Maark, T.; Ghatak, K.; Ahuja, R.; Pal, S., Scandium-Decorated MOF5 as

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Potential Candidates for Room-Temperature Hydrogen Storage: A Solution for the Clustering Problem in MOFs. *J. Phys. Chem. C* **2012**, 116, 17336-17342. (IF=4.18)

**03.** Kumari, N.; **Dixit, M.**; Roesky, H. W.; Mishra, L., Thiocyanato Bridged Heterodinuclear Complex  $[Cu(Bpy)_2(-NCS)Ru(Bpy)_2(NO_3)](PF_6)_2$  and Its Binding with Cd (II), Hg (II), Pb (II) and Ag (I) Ions. *In Chemistry for Sustainable Development*, Springer: **2012**; pp 231-247.

**02.** **Dixit, M.**; Maark, T. A.; Pal, S., *Ab-Initio* and Periodic DFT Investigation of Hydrogen Storage on Light Metal-Decorated MOF-5. *Int. J. Hydrogen Energy* **2011**, 36, 10816-10827. (IF=4.93)

**01.** Kumari, N.; Prajapati, R.; **Dixit, M.**; Mishra, L., Selective Binding of Benzoquinone with a Pt(II)-Cyclophane Constructed on the Skeleton of N, N'-Bis (Salicylidene)- PPhenylenediamine: Synthesis and Spectroscopic Studies. *Ind. J. Chem. A* **2009**, 48, 1644-1651.

## Awarded Proposals

- **SERB Core Research Grant, Dec -2020**, "Making Sodium the new Lithium: Stabilizing Oxygen Redox in High-Energy Sodium-ion Batteries through Accelerating Materials Discovery", Role: PI peer-reviewed **for three years**
- **Matching Grant**, "Research Matching Grant", Role: PI **for three years**
- **The PBC Fellowship Program for Outstanding Post-Doctoral Researchers**, "Lithiated Metal Oxide-based Cathode Materials for Li-ion Batteries", Role: Researcher, peer-reviewed
- **Extreme Science and Engineering Discovery Environment (XSEDE) Start-up Proposal**, National Science Foundation (NSF), "Insights into  $CO_2$  Reduction over Transition Metal Carbide Catalysts" was selected and awarded 50000 core hours, Role: PI, peer-reviewed
- **Research Proposal** " $CO_2$  Hydrogenation to Methanol over  $Co_2C$  Catalyst" was awarded (Funding from US Naval Research Lab, Role: Researcher (contributed to proposal writing), PI: Prof. Giannis Mpourmpakis

## Experimental Collaboration

- Close coloration with leading Li/Na-ion battery research groups (Prof. Doron Aurbach, Bar Ilan University, and Prof. Linda Nazar, University of Waterloo)
- Worked on different collaborative projects with global chemical companies like BASF (www.basf.com) and Lubrizol (www.lubrizol.com)

## Computational Expertise

Computational Material Sciences (First principles periodic DFT)

**Expert on codes:**, Vienna *Ab-initio* Simulations Package (VASP) and CP2K.

- DFT, Ab-initio MD, Free Energy Sampling, Surfaces, CI-NEB, Interfaces, Band-structures, Electronic Structure (DOS), COHP/COOP;
- Atomistic simulations using GULP

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### High-throughput computing and Machine Learning

**Expert on codes:**, *pymatgen, Aflow and ASE.*

- Developing expertise in automate,
- Developing expertise in matminer, automatminer, FireWorks

### Electronic Structure Theory (*Ab-initio and DFT*)

**Expert on codes:** , *Gaussian, CP2K, GAMESS, Turbomole, deMon2K.*

- Determination of the transition states and mechanistic pathways
- Investigation of biosynthetic pathways

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## Programming Experiences

Python, FORTRAN, Bash scripting, Cluster Administration

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## Select Oral Presentations

1. Delivered an Invited Talk at NAMMA Psi-k Workshop, New Approaches and Machine learning Methods for Ab initio calculations, (**Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR) and IISc Bangalore**) **July 24-28, 2023, Bengaluru, India**
2. Delivered an Invited talk at the 26th International Workshop on Quantum Systems in Chemistry, Physics, and Biology (QSCP-XXVI) will be held in **Jaipur, Rajasthan, India on October 14-20, 2023**
3. Delivered an Invited Talk on "Sodium-ion Batteries" at the 15th National Conference on Solid State Ionics (NCSSI-15) December 2-4, 2023 at **Department of Physics, Banaras Hindu University, Varanasi**
4. Delivered an invited talk on Computational Modeling for Sustainable Energy - Designing Superior Materials and Catalysts for a Cleaner Future, at the Department of Physics (28th Nov, 2023) at the **SRM Institute of Science and Technology, Kattankulathu**
5. Delivered an Invited Hands-on session on Machine Learning - Computational Modeling for Sustainable Energy - Designing Superior Materials and Catalysts for a Cleaner Future at the Department of Physics (28th Nov, 2023) at the **SRM Institute of Science and Technology, Kattankulathu**
6. Invited talk: Designing Improved Positive Electrode Materials for High-Energy Sodium- Ion Batteries Through Electronic Structure Tuning. a national conference on "Energy Materials and Devices" , **IIT Jodhpur, December 16 – 18, 2022.**
7. Delivered an Invited talk "Designing Improved Positive Electrode Materials and Electrocatalysts Through Electronic Structure Tuning" Designing Catalysts on Computers (DCC22), **IACS Kolkata on December 02-03, 2022**
8. Invited Talk: Computational Modelling for Sustainable Energy: Designing Superior Materials and Catalysts for a Cleaner Future. A Two-day DST-SERB sponsored hands-on training workshop Density Functional Theory (DFT) Modelling and Machine Learning in Chemistry, **Ramaiah University of Applied Sciences (RUAS), 12 -13, April 202**
8. Delivered an Invited talk "Designing Improved Positive Electrode Materials for Sodium-ion Batteries Through Electronic Structure Tuning" International conference on recent advances in renewable energy (CARE-2023), **HRI Pryagraj, February 2-4 2023.**
10. Delivered an invited lecture on "*Tutorial session on Computational Chemistry*" **Tools and**

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**Techniques in Chemical Sciences (2021) IUST Jammu and Kashmir, India**

11. Delivered an invited talk on "Elucidating the origin of capacity fading of Ni-rich layered oxide-based positive electrode materials for Li-ion batteries" **Advanced Materials for Better Tomorrow (AMBT 2021): IIT BHU, India**

12. Delivered an invited talk on "Elucidating the origin of capacity fading of Ni-rich layered oxide-based positive electrode materials for Li-ion batteries" **International Conference on Materials Genome (ICMG-2020) Organized by SRM University – AP, India**

12. Delivered an oral talk on "*Elucidating the role of oxygen coverage in CO<sub>2</sub> reduction on Mo<sub>2</sub>C*" **ACS Spring Meeting (2018)**, New Orleans, LA, USA

14. Delivered an oral talk on "*Understanding the C-H Activation and Dehydrogenation Mechanisms of Alkanes on Metal Oxides*" **AICHE Annual Meeting (2017)**, Minneapolis, MN, USA

15. Delivered an oral talk on "*Developing structure-activity relationships in the dehydrogenation of alkanes on oxides*" **ACS Fall meeting (2017)**, Washington D.C., USA 16. Delivered an invited Keynote talk on "*Computational Insights into the Electrochemical and Thermodynamic Properties, and Degradation Mechanisms of Ni-rich NCMs*" at **International conference on computational materials science "ICAPMMP-IV"**, Indian Institute of Technology (IIT) Kharagpur, Nov 5-7, 2016

17. Delivered an oral talk on "*Electrochemical and Kinetic Studies of  $\text{LiNi}_{0.50}\text{Co}_{0.2}\text{Mn}_{0.3}\text{O}_2$  using Density Functional Theory*" at **IsraElectrochemistry conference**, Ben-Gurion University, Israel, Sept 15, 2015.

18. Delivered invited talk on "*Scandium-Decorated MOF-5 as Potential Candidates for Room-Temperature Hydrogen Storage*" at **The Second Bilateral Indo-French Symposium on "Catalysis for Sustainable and Environmental Chemistry"** Lille, France, July 11-13, 2012.

19. Delivered Oral talk on "*Scandium-Decorated MOF-5 as Potential Candidates for Room-Temperature Hydrogen Storage*". **Divisional Day Conference**, National Chemical Lab, Pune, 30 November 2012.



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