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*.

April 2019–Dec 2022 **Assistant Professor**, *Lovely Professional University*, Phagwara, *India*.

Adyar – Chennai-60020 – India
+7814742085 • *+91 (44) 2443 7150*
muditdixit@clri.res.in, dixitmuditk@gmail.com • *dixitmudit.in/*

Present Academic Appointment

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

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=24, Total citations=3230+

50. Gupta, N. Halder, S. Behere, R.P., Singh, P. Kanungo, S. **Dixit, M.***, Chanchal Chakraborty*, and Biplab Kumar Kuila* Boosting CO2 Activation and Reduction by Engineering the Electronic Structure of Graphitic Carbon Nitride through Transition Metal-Free Single-Atom Functionalization textitACS 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 CO2 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 -Al2O3 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)**

Adyar – Chennai-60020 – India
+7814742085 • +91 (44) 2443 7150
muditdixit@clri.res.in, dixitmuditk@gmail.com • dixitmudit.in/

44. Rasool, A.; Anis, I.; **Dixit, M.**; Maibam, A.; Hassan, A.; Krishnamurty, 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 selanyl 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)**

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.; Kunnikuruvan, 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**; Daean, 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. Kostetskyy, 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; Kostetskyy, 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 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)**.

Adyar – Chennai-60020 – India
+7814742085 • ☎ +91 (44) 2443 7150
muditdixit@clri.res.in, dixitmuditk@gmail.com • dixitmudit.in/

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)**

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)**

Adyar – Chennai-60020 – India
+7814742085 • +91 (44) 2443 7150
muditdixit@clri.res.in, dixitmuditk@gmail.com • dixitmudit.in/

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 $Zn_{1x}Mn_xO$ 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 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**

Adyar – Chennai-60020 – India
+7814742085 • *+91 (44) 2443 7150*
muditdixit@clri.res.in, dixitmuditk@gmail.com • *dixitmudit.in/*

- **Matching Grant, LPU**, "Research Matching Grant, LPU", 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

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

Programming Experiences

Python, FORTRAN, Bash scripting, Cluster Administration

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,**

Adyar – Chennai-60020 – India
+7814742085 • +91 (44) 2443 7150
muditdixit@clri.res.in, dixitmuditk@gmail.com • dixitmudit.in/

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 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 CO2 reduction on Mo2C"* **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* $LiNi_{0.50}Co_{0.2}Mn_{0.3}O_2$ *using Density Functional Theory"* at **IsraElectrochemistry conference**, Ben-Gurian 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.

(Mudit Dixit)

Adyar – Chennai-60020 – India
+7814742085 • ☎ +91 (44) 2443 7150
✉ muditdixit@clri.res.in, dixitmuditk@gmail.com • dixitmudit.in/