

# 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.**  
Accelerated Catalysis Discovery Using Advanced Computational and Machine Learning Methods for Alkane Dehydrogenation, CO Reduction, and 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/Na-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 (rechargeable batteries) using First principles-based methods
- Machine Learning for Accelerated Catalyst Discovery
- Computational Heterogeneous electroCatalysis

## Publications, h-index=27, Total citations=4477+

63. Maurya, A.; Singh, P.; Dixit\*, M.; Kuila, B. K.\* Engineering Triazine-Based Conjugated Polymer Networks for Boosting Electrocatalytic Hydrogen Evolution Reactions *ACS Appl. Energy Mater.* **2025**, (<https://doi.org/10.1021/acsaem.5c00638>)
62. Maurya, A.; Gupta, N.; Singh, P.; Bhutani, N.; Anamika; Koner, R. R.; Dixit\*, M.; Kuila, B. K.\* Nitrogen- and Sulfur-Enriched Conjugated Polymer Network as an Electrocatalyst for the Oxygen Reduction Reaction and as a Cathode Material for Zinc–Air Batteries. *ACS Appl. Energy Mater.* **2025**, 8, 14408–14416.
61. Bhise, R.; Kadrekar, R.; Singh, P.; Nidamanuri, N.; Arte, P.; Nath, P.; Wang, Y.; Sheikh, A. D.; Dixit, M.; Sahu, S. P. Facile Single-Step Synthesis of PVP-Stabilized Ru NPs for Electrochemical Hydrogen Generation. *Energy Fuels* **2025**, 39, 43, 20896–20907.
60. Kumar, S.; Maurya, A. K. R.; Dixit, M.\* Unravelling the Catalytic Activity of Dual-Metal Doped N6-Graphene for Sulfur Reduction via Machine Learning-Accelerated First-Principles Calculations. arXiv Preprint **2025**, arXiv:2510.15397.
59. Sudheer Kumar Gogulaa, Vasantha A. Gangadadharappa, Priti Singhb,Vinoth Kumar Jayarama, **Dixit, M.** Annigere S. Prakash. Moisture and Air-Stable Cation Disordered O3-Type Layered Cathode for Sodium-Ion Batteries: Experimental and First-Principles Study *J. Mater. Chem. A*, **2025**, 13, 38335-38349
58. Priti Singh, Sahil Kumar, **Dixit, M.\***. Understanding the Effect of Metal-Oxygen Bond Covalency on Anionic Redox Activity of Na-ion based Cathode Materials through First-Principles *Journal of Chemical Sciences* **2025** (*just accepted*)

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**56.** Amrita Gogoi, **Dixit, M.**, S Pal,. Modelling an Fe-III High-Valent Pincer-type Transition Metal Complex for Dehydrogenation of Ammonia-Borane *Chemistry–An Asian Journal* **2025** e202401976 (IF=4.3)

**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** (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**, 128, 37, 7804–7815(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 Irulkuvajjula, 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 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)

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- 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.; Krishnamurty, S.; Dar, M. A., Tantalum based single, double, and triple atom catalysts supported on gC<sub>2</sub>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 indanedi one 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<sub>2</sub>C* 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<sub>1-x-y</sub>Co<sub>x</sub>Mn<sub>y</sub>O<sub>2</sub>* and *LiNi<sub>1-x-y</sub>Co<sub>x</sub>Al<sub>y</sub>O<sub>2</sub>*. *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

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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 *njp 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)**

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- 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; Taliander, M; Grinblat, J; Sclar, H; Breuer, O; Julien, C.M; Munichandraiah, N; Kovacheva, 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.; Taliander, 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**,**

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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 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.

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## 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 Mpormpakis

## Experimental Collaboration

- Close collaboration 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](http://www.bASF.com)) and Lubrizol ([www.lubrizol.com](http://www.lubrizol.com))

## Programming Experiences

Python, FORTRAN, Bash scripting, Cluster Administration

## Method and Code Development

- **PACE (Precise and Accurate Configuration Evaluation)** Developed an open-source tool PACE (Precise and Accurate Configuration Evaluation), a machine-learning-accelerated framework that couples ML Interatomic Potentials (MLIPs) with DFT to systematically explore adsorption configurations and energetics on complex catalytic surfaces. PACE is general and transferable; it can screen any catalyst-host system, far beyond just Li-S batteries. <https://github.com/dixitmudit/PACE>.
- **AutoML-Reg: Automated Machine Learning Regression Framework** Designed an in-house AutoML pipeline that automatically performs ML regression using multiple algorithms including CatBoost, Gradient Boosting, Random Forest, XGBoost, and Support Vector Regression. The tool reads features and target properties directly from Excel (XLS/XLSX), performs preprocessing, feature scaling, model training, hyperparameter optimization, validation, and generates comparative performance metrics for materials-property prediction.
- **DFT-MLIP Integrated Simulation Pipelines** Developed multi-scale modeling workflows combining DFT, machine-learning interatomic potentials, molecular dynamics for accelerated screening of Ni-rich and Na-rich cathode materials and catalytic systems.

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## Select Invited Talks, Keynotes Talks, Workshops, and Training Sessions

- Delivered a Pedagogical Keynote Talk on “*Accelerating Materials Discovery for Electrochemical Energy Storage via Computation and Machine Learning*” at the 5-Day Short-Term Training Program (STTP) on **Applications of Machine Learning in Chemical Process Outcomes Prediction (STTP-ML)**, SRM Institute of Science and Technology, Kattankulathur.
- Delivered a Keynote Talk and conducted a Hands-on Training Program on “*Fundamentals of Machine Learning for Materials Discovery*” at the Faculty Development Program, **VIIT Vellore, 18–22 August 2025**.
- Delivered a Pedagogical Keynote Talk on “*Machine Learning Approaches in Electrochemical Energy Storage: An Introduction*” at the Faculty Development Program on “**Experimental and Computational Synergies in Environmental Applications,**” VIT Vellore, **8–12 September 2025**.
- Delivered an invited talk at the **International Conference on Sustainable Batteries (ICSB-2025)**, TCG-CREST, Kolkata, 24–27 February 2025.
- Delivered an invited talk at the **International Conference on Sustainable Catalysis: Synthesis, Theory, and Applications (SusCat-STA 2024)**, Udaipur, 22–26 July 2024.
- Delivered an invited seminar in the **Monthly Seminar Series**, Department of Chemical Engineering, IIT Madras, 20 September 2024.
- Delivered an invited talk titled “*Accelerating Materials Discovery for Catalysis and Electrochemical Energy Storage*” at **Current Trends in Theoretical Chemistry (CTTC-2024)**, 28 September 2024.
- Delivered an invited talk titled “*Accelerating Cathode Material Discovery for Next-Generation Sodium-ion Batteries Using First-Principles Calculations and Machine Learning Potentials*” at the **National Meeting on Sodium-ion Batteries (NMSB-1)**, IIT Bombay, 4–6 October 2024.
- Delivered an invited talk at **Physics and Chemistry of Atomic, Molecular, and Condensed Matter Systems (PCAMC-2024)**, IISER Kolkata, 11–14 December 2024.
- Delivered an invited talk titled “*Advanced Computational Approaches for Electrochemical Energy Storage Material Design*” at the **UGC–Malaviya Mission Teacher Training Centre (MM-TTC)**, Central University of Jammu, organized with the Department of Physics and Astronomical Sciences and the Department of Chemistry and Chemical Sciences, 10–23 December 2024.
- Delivered an Invited Talk at the NAMMA Psi-k Workshop, “*New Approaches and Machine Learning Methods for Ab initio Calculations,*” **JNCASR and IISc Bangalore, 24–28 July 2023, Bengaluru, India.**
- Delivered an Invited Talk at the **26th International Workshop on Quantum Systems in Chemistry, Physics, and Biology (QSCP-XXVI)**, Jaipur, Rajasthan, 14–20 October 2023.
- Delivered an Invited Talk on “*Sodium-ion Batteries*” at the **15th National Conference on Solid State Ionics (NCSSI-15)**, Department of Physics, Banaras Hindu University, Varanasi, 2–4 December 2023.
- Delivered an invited talk on “*Computational Modeling for Sustainable Energy – Designing Superior Materials and Catalysts for a Cleaner Future*” at the **Department of Physics, SRM Institute of Science and Technology, Kattankulathur**, 28 November 2023.
- Delivered an Invited Hands-on Session on “*Machine Learning and Computational Modeling for Sustainable Energy*” at the **Department of Physics, SRM Institute of Science and Technology, Kattankulathur**, 28 November 2023.
- Delivered an Invited Talk: “*Designing Improved Positive Electrode Materials for High-Energy*

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*Sodium-Ion Batteries Through Electronic Structure Tuning*" at the National Conference on **Energy Materials and Devices**, IIT Jodhpur, 16–18 December 2022.

- Delivered an Invited Talk: "*Designing Improved Positive Electrode Materials and Electrocatalysts Through Electronic Structure Tuning*" at **Designing Catalysts on Computers (DCC22)**, IACS Kolkata, 2–3 December 2022.
- Delivered an Invited Talk: "*Computational Modelling for Sustainable Energy: Designing Superior Materials and Catalysts for a Cleaner Future*" at the DST–SERB sponsored Hands-on Workshop on **Density Functional Theory (DFT) Modelling and Machine Learning in Chemistry**, Ramaiah University of Applied Sciences (RUAS), 12–13 April 2022.
- Delivered an Invited Talk: "*Designing Improved Positive Electrode Materials for Sodium-ion Batteries Through Electronic Structure Tuning*" at the **CARE-2023 International Conference on Renewable Energy**, HRI Prayagraj, 2–4 February 2023.
- Delivered an invited lecture on "*Tutorial Session on Computational Chemistry*" at **Tools and Techniques in Chemical Sciences (2021)**, IUST Jammu Kashmir.
- Delivered an invited talk on "*Elucidating the Origin of Capacity Fading of Ni-rich Layered Oxide Positive Electrode Materials for Li-ion Batteries*" at **Advanced Materials for Better Tomorrow (AMBT-2021)**, IIT BHU, India.
- Delivered an invited talk on "*Elucidating the Origin of Capacity Fading of Ni-rich Layered Oxide Positive Electrode Materials for Li-ion Batteries*" at the **International Conference on Materials Genome (ICMG-2020)**, SRM University–AP, India.
- Delivered an oral talk on "*Elucidating the Role of Oxygen Coverage in CO<sub>2</sub> Reduction on Mo<sub>2</sub>C*" at the **ACS Spring Meeting 2018**, New Orleans, LA, USA.
- Delivered an oral talk on "*Understanding the C–H Activation and Dehydrogenation Mechanisms of Alkanes on Metal Oxides*" at the **AIChE Annual Meeting 2017**, Minneapolis, MN, USA.
- Delivered an oral talk on "*Developing Structure–Activity Relationships in the Dehydrogenation of Alkanes on Oxides*" at the **ACS Fall Meeting 2017**, Washington, D.C., USA.
- Delivered an invited Keynote Talk on "*Computational Insights into the Electrochemical and Thermodynamic Properties and Degradation Mechanisms of Ni-rich NCMs*" at the **International Conference on Computational Materials Science (ICAPMMP-IV)**, IIT Kharagpur, 5–7 November 2016.
- Delivered an oral talk on "*Electrochemical and Kinetic Studies of LiNi<sub>0.50</sub>Co<sub>0.2</sub>Mn<sub>0.3</sub>O<sub>2</sub> using Density Functional Theory*" at the **IsraElectrochemistry Conference**, Ben-Gurion University, Israel, 15 September 2015.
- Delivered an invited talk on "*Scandium-Decorated MOF-5 as Potential Candidates for Room-Temperature Hydrogen Storage*" at the **Second Indo–French Symposium on Catalysis for Sustainable and Environmental Chemistry**, Lille, France, 11–13 July 2012.
- Delivered an oral talk on "*Scandium-Decorated MOF-5 as Potential Candidates for Room-Temperature Hydrogen Storage*" at the **Divisional Day Conference**, National Chemical Laboratory (NCL), Pune, 30 November 2012.



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