Mudit Dixit

Department of Chemical Engineering, University of Pittsburgh

Academic Qualifications

2008-2013 **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–Current **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, 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

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)

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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

- **Heterogeneous Catalysis**
- **Electrochemical Energy Storage**
- **Enzyme Catalysis**

Publications

1. 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.

2. 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., **2017**, 83, 1176-1184.*

3. 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*

4. 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.

5. 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.

6. 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 **(Featured on the front cover, selected as a hot article of 2017)**.

7. 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.

8. 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.

9. 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 **(Selected by the editor and featured on the front cover)**.

10. 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.

11. 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.

12. 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

13. 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.

14. 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.

15. 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.

16. 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 **Incuded in a themed collection "2016 most accessed PCCP articles"**.

17. 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.

18. 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.

19. 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.

20. 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.

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21. 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.

22. 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.

23. 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.

24. 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.

25. 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.

26. 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.

27. 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. *Indian Journal of Chemistry A* **2009**, 48, 1644-1651.

28. 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.

29. Chakraborty, A.; **Dixit, M.**; Major; D.T., Accurate Cathode Properties of $LiNiO_2$, $LiCoO_2$, and $LiMnO_2$ Using the SCAN Meta-GGA Density Functional *arXiv:1805.00642*: **2018**.

30. 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. **(2018)** *Purinergic Signaling,* **2018**, 14,3, 271–284.

Under review

1. Dixit, M; Kostetskyy, P; Mpourmpakis, G. Structure-Activity Relationships in Alkane Dehydrogenation on $\gamma - Al_2O_3$: Site-Dependent Reactions *(ACS Catalysis, under review)*.

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Awarded Proposals

- **The PBC Fellowship Program for Outstanding Post-Doctoral Researchers**, "Lithiated Metal Oxide-based Cathode Materials for Li-ion Batteries", Role: Researcher (Led the proposal writing), 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, Role: PI, peer-reviewed
- **Research Proposal** "CO_2 Hydrogenation to Methanol over Co_2C Catalyst" was selected and awarded $\$24,000$ (Funding from US Naval Research Lab, Role: Researcher(Led the proposal writing), PI: Dr. Giannis Mpourmpakis, peer-reviewed

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- **The Partnership for Advanced Computing in Europe (PRACE) proposal No. 2010PA3025 (2015)** "Computational Design of Ni-rich, Layered Oxide Based Positive Electrode Materials" was selected and awarded 300000 core hours, Role: Researcher(Led the proposal writing), PI: Prof. Dan T. Major, peer-reviewed
- **Led: PRACE proposal No. 2010PA3048 (2015)** "Study of Dynamical Effects in Enzyme Catalysis of Dihydrofolate Reductase and Dormate Dehydrogenase." was selected and awarded 150000 core hours, Role: Researcher, (Led the proposal writing) PI: Prof. Dan T. Major, peer-reviewed

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 (Plane wave 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

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

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

- Determination of the transition states and mechanistic pathways
- Multi-scale modeling (QM/MM) with CHARMM, investigation of biosynthetic pathways, force field development

Programming Experiences

FORTRAN 90, Bash scripting, Python, Cluster Administration

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List of Select Talks and Posters

1. Delivered an oral talk on *"Elucidating the role of oxygen coverage in CO2 reduction on Mo2C"* **ACS Spring Meeting (2018)**, New Orleans, LA, USA
2. 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
3. Delivered an oral talk on *"Developing structure-activity relationships in the dehydrogenation of alkanes on oxides"* **ACS Fall meeting (2017)**, Washington D.C., USA
4. 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
5. 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.
6. 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.
7. Delivered *Oral talk* on *"Ab-initio and periodic DFT investigation of hydrogen storage on light metal-decorated MOF-5"*. **HYPOMAP meeting**, CLRI Chennai, 12-13 July 2011.
8. Presented *poster* on *"Understanding the C-H Activation and Dehydrogenation Mechanisms of Alkanes on* γ*–Alumina"* at **Pittsburgh-Cleveland Catalysis Society Annual Meeting (2017)**, Akron OH, USA, May 25, 2017
9. Presented poster "Ab-initio study of cathode materials for lithium-ion batteries" in 2015 **CECAM Symposium of the Lise Meitner - Minerva Center for Computational Quantum Chemistry**, 3 May 2015. Tel Aviv University, Israel
10. Presented poster on *"Understanding the cathode materials for lithium-ion batteries using first principles"*, in **IsraElectrochemistry 2014**, Tuesday, September 16, 2014, Technion, Israel
11. Attended *Hands-on DFT codes from Julich*, **CECAM juDFT Tutorials** on Forshchugzentrum Julich, Germany, 22-26 September 2014

Student Supervision

2017–Current: Currently supervising one undergraduate student (J.W.E.) and one masters student (R.T.). Supervised two undergraduate students (P.T.D and M.C.) and one Masters Student (X.P.), University of Pittsburgh, USA

2014–2016: Supervised two undergraduate students (B.D. and S.B.) and two senior research students (S.D. and A.C.), Bar Ilan University, Israel

2010–2010: Supervised lab course on "Scientific Computing" at the Indian Institute of Science Education and Research (IISER) Pune, (2010)

Academic Service

- Serving as a referee in 6 international journals including J. Electrochem. Soc., ACS Catal. (https://publons.com/author/1330156/mudit-dixitprofile)

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- Serving as a Review Editor for "Frontiers in Chemistry" Journal (Electrochemistry Section)
- Chaired two sessions at ACS Spring meeting (2018), New Orleans, LA, USA
- Chaired two sessions at ACS Fall meeting (2017), Washington D.C., USA
- Served as one of the editors of 'DHAWANI' NCL's first annual magazine. (2012)
- Served as the General Secretary (2009-2010) of the 'Hall of residence I', National Chemical Laboratory, India.

(Mudit Dixit)

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