Mudit Dixit

Department of Chemical Engineering, University of Pittsburgh

Academic Qualifications

2008-2013 **Doctor of Philosophy**, *Computational and Materials 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. (7.34 CGPA)

2003-2006 **Bachelor of Science (Chemistry, Physics and Mathematics)**, *India*.
Rohilkhand University, Shahjahanpur, secured first rank in the college. (74.22%)

Research Experience

Jan 2017– **Postdoctoral Fellow**, *University of Pittsburgh*, Pittsburgh, *USA*.
Structure activity relationships for 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 Fellow**, *Bar-Ilan University*, Ramat Gan, *Israel*.
Design and investigation of cathode materials for Li-ion batteries using ab-initio and DFT methods with a close collaboration with the experimental group of Prof. Doron Aurbach and BASF (Chemical Company).
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

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2008 **Qualified Graduate Aptitude Test in Engineering (GATE)**, *India*.
Conducted by the Indian Institute of Technology (IIT) (96.22 percentile)

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

- Computational Materials Chemistry
- Heterogeneous catalysis
- Electrochemical energy storage, and enzyme catalysis, hybrid QM/MM

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 (7), 2430–2437 **IF=2.19**

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*, **(IF=4.80)**

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* **(IF= 30.06)**

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 **(IF= 4.48)**

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 **(IF=21.87)**

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) (IF= 5.773)**

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 **(IF= 11.38)**

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 **(IF=4.857)**

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 **(IF= 3.259, 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 (1), pp 812–818 **(IF= 11.38)**

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 **(IF=9.89)**

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 **(IF=9.93)**

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. **(IF= 2.88)**

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. **(**IF= 2.002)

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 (20), 4640- 4653. **(IF= 3.42)**

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 **(IF= 3.90)**

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 **(IF= 5.16)**

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. **(IF= 1.860)**

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. **(IF= 4.48)**

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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 **(IF= 3.90)**

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. **(IF= 3.259)**

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 **(IF= 6.25)**

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. **(IF=4.22)**

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 **(IF=4.22)**

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 **(IF= 4.48)**

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. **(IF=0.9)**

27. Kumari, N.; Prajapati, R.; **Dixit, M.**; Mishra, L., Selective Binding of Benzoquinone with a Ptii-Cyclophane Constructed on the Skeleton of N, N'-Bis (Salicylidene)- PPhenylenediamine: Synthesis and Spectroscopic Studies. *Indian Journal of Chemistry A* **2009**, 48, 1644-1651. **(IF= 0.49)**

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* Accepted.

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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)*

Awarded Proposals

- **Led: Research Proposal** "CO_2 Hydrogenation to Methanol over Co_2C Catalyst" was selected and awarded $\$24,000$ (Funding from US Naval Research Lab, with Dr. Giannis Mpourmpakis)

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- **Led: PRACE proposal No. 2010PA3025 (2015)** "Computational Design of Ni rich, Layered Oxide Based Positive Electrode Materials" was selected and awarded 300000 core hours.
- **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
- **Contributed: Extreme Science and Engineering Discovery Environment (XSEDE) Proposal**, National Science Foundation (NSF), was selected and awarded SUs worth $\$32,355.54$

Experimental Collaboration

- Close coloration with global leaders in Li/Na-ion battery research (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 investigations)

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

- Determination of Transition States and Mechanistic Pathways
- Multi-scale modelling (QM/MM) with CHARMM, investigation of biosynthetic pathways, force field developments

Programming Experiences

FORTRAN 90	*Proficient*
Bash scripting	*Proficient*
Python	*Intermediate*
Cluster Administration	*Intermediate*

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Selected 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 to 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 *"Underatanding the cathode materials for lithium ion batteries using first principles"*, in **IsraElectrochemistry 2014**, Tuesday, Sept. 16 2014, Technion, Israel
11. Attended *Hands-on DFT codes from Julich*, **CECAM juDFT Tutorials** on Forshchugzentrum Julich, Germany, 22-26 September, 2014

Students Supervision

- Currently supervising two undergraduate students and one masters student
- Supervised two undergraduate student at Bar-Ilan University, Israel (2015-2016)
- Supervised lab course on "Scientific Computing" at the Indian institute of science education and research (IISER) Pune, (2010)

Academic Service

- Referee in 6 international journals: J. Electrochem. Soc., ACS Catal., Bull. Mater. Sci., Int. J. Mol. Sci., Batteries, and Energies
- Judged PQI-2018 poster session
- Chaired two sessions at ACS Spring meeting (2018), New Orleans, LA, USA
- Chaired two sessions at ACS Fall meeting (2017), Washington D.C., USA

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- Served as one of the editor of 'DHAWANI' NCL's first annual magazine. (2012)
- Served as General Secretary (2009-2010) of the 'Hall of residence I', National Chemical Laboratory, India.

(Mudit Dixit)

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