

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

Under review/revision

33. Dixit, M; Kostetskyy, P; Mpourmpakis, G. Structure-Activity Relationships in Alkane Dehydrogenation on $\gamma - Al_2O_3$: Site-Dependent Reactions (*ACS Catalysis*, under minor revision).
32. Kostetskyy, P; Carly, N; Dixit, M; Mpourmpakis, G. Understanding Alkane Dehydrogenation through Alcohol Dehydration on $\gamma - Al_2O_3$ (*Industrial & Engineering Chemistry Research*, under review).
31. Cholewinski, M; Dixit, M; Mpourmpakis, G. Computational Study of Methane Activation on $\gamma - Al_2O_3$ (*ACS Omega*, under review).

Published

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.
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*, (Accepted), **2018**.
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.
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
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.

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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.
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.
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.
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 (**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 (**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.
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.
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
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.
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.

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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.
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 **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.
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.
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.
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.
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.
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.
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.
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.
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.

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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.

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

- **The PBC Fellowship Program for Outstanding Post-Doctoral Researchers**, "Lithiated Metal Oxide-based Cathode Materials for Li-ion Batteries", Role: Researcher (Led proposal writing), peer-reviewed **Funding:** \$100,776
- **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
- **The Partnership for Advanced Computing in Europe (PRACE) proposal No. 2010PA3025 (2015)** "Computational Design of Ni-rich, Layered Oxide Based Positive Electrode Materials" was awarded 300000 core hours, Role: Researcher (contributed to 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 awarded 150000 core hours, Role: Researcher, (contributed to 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

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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

Participation in Conferences/Presentations

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}O₂ using Density Functional Theory*" at **IsraElectrochemistry conference**, Ben-Gurion 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 "*Scandium-Decorated MOF-5 as Potential Candidates for Room-Temperature Hydrogen Storage*". **Divisional Day Conference**, National Chemical Lab, Pune, 30 November 2012.
8. Delivered Oral talk on "*Ab-initio and periodic DFT investigation of hydrogen storage on light metal-decorated MOF-5*". **HYPOMAP meeting-2011**, CLRI Chennai, 12-13 July 2011.
9. Delivered Oral talk on "*Hydrogen storage on Li-functionalized MOFs*". **HYPOMAP meeting - 2010**, Bhabha Atomic research Centre, Mumbai, 8-10 July 2010.
10. 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
11. 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
12. Presented poster on "*Understanding the cathode materials for lithium-ion batteries using first principles*", in **IsraElectrochemistry 2014**, Tuesday, September 16, 2014, Technion, Israel
13. Presented poster on "*Understanding the cathode materials for lithium-ion batteries using first principles*", in **IsraElectrochemistry 2014**, Tuesday, September 16, 2014, Technion, Israel
14. Presented poster on "*Comparative Study of hydrogen storage in MOF-5*", in **Changing Paradigms of Theoretical Computational Chemistry: From Atoms to Molecular Clusters, TCCC 2009**, Tuesday, December 18-20 2009, University of Pune, India

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15. Presented poster on "*Ab initio study of cathode materials for lithium ion batteries*", in **Isra-electrochemistry 2014**, Tuesday, September 16 2014, Indian Institute of technology, Kanpur, India
16. Presented poster on "*Ab initio study of cathode materials for lithium ion batteries*", in **Bar Ilan-Weizmann UCMRS Materials Science Student Conference**, Tuesday, Wednesday October 29, 2014, Bar Ilan University Israel
17. Presented poster on "*Transition Metal Oxides as Cathode Materials for Lithium ion Batteries*", in **Metal Oxide Material Discovery applications**, Thursday January 15, 2015, Hebrew University, Jerusalem, Israel
18. Presented poster on "*2015 Symposium of the Lise Meitner - Minerva Center for Computational Quantum Chemistry*", in **BINA Internal Conference**, Sunday May 3, 2015, Tel Aviv University, Israel
19. Presented poster on "*Computational study of $Ni_{0.5}Co_{0.2}Mn_{0.3}O_2$ as a cathode materials for lithium ion batteries*", in **BINA Internal Conference**, Monday February 9, 2015, Bar Ilan University, Israel
20. Presented poster on "*Classical and Quantum Modeling of Li and Na Diffusion in $FePO_4$* ", in **Isotopes2015** June 21-26, 2015 Jerusalem, Israel
21. Presented poster on "*Computational Insights to the Layered to Spinel transformation in Ni-rich NCMs*", in **The 17th Israel Materials Engineering Conference**, Monday February 1, 2016, Bar Ilan University, Israel
22. Presented poster on "*Transition Metal Oxides as Cathode Materials for Lithium ion Batteries*", in **Recent Advances in Computational Modeling for Energy Applications**, Tuesday July 7, 2015, Technion, Israel
23. Presented poster on "*Ab-initio and DFT investigations of Hydrogen storage*", in **Theoretical Chemistry Symposium 2010 (TCS10)**, Tuesday, December 08-12 2010, Indian Institute of technology, Kanpur, India
24. Presented poster on "*Comparative Study of hydrogen storage in MOF-5*", in **Changing Paradigms of Theoretical Computational Chemistry: From Atoms to Molecular Clusters, TCCC 2009**, Tuesday, December 18-20 2009, University of Pune, India
25. 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.) in the Mpourmpakis group in the Department of Chemical Engineering at the 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.) in the Major group in the Chemistry Department at Bar-Ilan University, Israel

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Teaching Experience

April 2017: Guest Lecturer

Delivered lectures on Ab-initio Molecular Dynamics and designed and led a training workshop for graduate students in the Mpourmpakis group in the Department of chemical and Petroleum Engineering, Pittsburgh, (attendees ~ 10).

November 2016: Guest Lecturer

Designed and instructed in a training workshop on Ab-initio calculations of electrode materials for Li-ion batteries using the Vienna Ab-initio simulation package (VASP) for graduate students in the Mechanical Engineering Department, Indian Institute of Technology (IIT) Kharagpur (attendees ~ 10).

December 2012: Guest Lecturer

Guest Lectured by invitation "Introduction to Quantum Chemistry" as a part of "Physical Chemistry" (B.Sc. – III Chemistry (Paper-III)) undergraduate course at S.S. College Shahjahanpur, India (attendees ~ 45).

August–November 2010: Teaching Assistant

Led problem solving sessions and graded the course in an undergraduate course of "scientific computing" at Indian Institute of Science (IISER), Pune (number of students ~ 40).

August–November 2011: Teaching Assistant

Led problem solving sessions and graded a graduate course of "Computational Chemistry" at Indian Institutes of Science Education and Research (IISER), Pune (number of students ~ 40).

Academic Service

- Serving as a referee in 7 international journals including J. Electrochem. Soc., ACS Catal. (<https://publons.com/author/1330156/mudit-dixitprofile>)
- 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.

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