

Mudit Dixit

Postdoctoral Fellow

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 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 the first rank in college. (74.22%)

Research Experience

- Jan 2017– **Post-Doctoral Fellow**, *University of Pittsburgh, Pittsburgh, USA*.
Structure activity relationships for dehydrogenation of alkanes on metals oxides, carbon dioxide reduction on metal carbides and design of new catalysts for methane activation.
Supervisor – Prof. Giannis Mpourmpakis
- 2014–2017 **Post-Doctoral Fellow**, *Bar-Ilan University, Ramat Gan, Israel*.
Design and investigation of cathode materials using ab-initio and DFT methods with the 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. 2008–2013)**, *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-current in aromatic molecules.
Supervisor – Prof. M.M. Balakrishna Rajan

Awards and Fellowships

- 2014 **Planning and Budgeting Committee (PBC) Post-doctoral fellowship**, *Israel*.
A fellowship program for outstanding post-doctoral researchers from China and India in Israeli universities

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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 and D organization
- 2008 **Qualified National Eligibility Test (NET)**, *India*.
Conducted University Grant Commission (UGC) and CSIR

Area of Interest

- Computational Materials Chemistry
- Heterogeneous catalysis
- Electrochemical and hydrogen 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* (just accepted) **2018**
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.*, **83**, 1176-1184, **(2017) (IF=4.85)**
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). **(IF= 29.51)**
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), pp 22628–22636 **(IF= 4.536)**
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= 16.721)**
6. **Dixit, M.**; Peng, X.; Porosoff, M. D.; Willauer, H.D.; Mpourmpakis, G.; Elucidating the role of oxygen coverage in CO₂ 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= 10.614)**
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)**

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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= 10.614**)
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=9.466**)
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= 8.867**)
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= 2.793**)
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= 3.564**)
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= 4.123**)
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= 5.317**)
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= 4.536**)

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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= 4.123)
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= 6.259)
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=3.582)
24. 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=3.582)
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= 4.536)
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.

Under review/Communicated Manuscripts

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

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Awarded Proposals

- **Lead: PRACE proposal No. 2010PA3025 (2015)** "Computational Design of Ni rich, Layered Oxide Based Positive Electrode Materials" was selected and awarded 300000 core hours.
- **Lead: 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 one of the global leaders in Li ion battery research (Prof. Doron Aurbach, Bar Ilan University and Prof. Linda Nazar, University of Waterloo)
- Worked for different project with global chemical company 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.*

- Ab-initio MD, Free energy sampling, surfaces, CI-NEB, interfaces, supercells, 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

FORTTRAN 90	<i>Proficient</i>
Bash scripting	<i>Proficient</i>
Python	<i>Intermediate</i>
Cluster Administration	<i>Intermediate</i>

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*

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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 Students
- 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)

Leadership

- Chaired two sessions at ACS Fall meeting (2017), Washington D.C. USA
- Chaired two sessions at ACS Spring meeting (2018), New Orleans, LA, USA
- Served as 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.

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