Mudit Dixit | Postdoctoral Fellow

University of Pittsburgh, United States – Department of Chemical and Petroleum Engineering

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Computational chemistry, Catalysis and Energy Storage

Awards and Fellowships

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

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

Junior Research Fellowship (JRF), India *2008*
Awarded by Council of Scientific and Industrial Research (CSIR), India, a premier national R and D organization

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

Research Experience

University of Pittsburgh **Pittsburgh**
Post-Doctoral Fellow, USA *Jan 2017–*
Structure activity relationships for dehydrogenation of alkanes on metals oxides, carbon dioxide reduction on metal carbides and new catalysts for OER and electrochemical splitting of water.
Supervisor – Prof. Giannis Mpourmpakis

Bar-Ilan University **Ramat Gan**
Post-Doctoral Fellow, Israel *2014–2017*
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

CSIR-National Chemical Laboratory **Pune**
Senior Research Fellow (Ph.D. 2008-2013), India *2010–2013*
Ab-*initio*, DFT and molecular dynamics investigations of hydrogen storage materials.
Supervisor – Prof. Sourav Pal

CSIR-National Chemical Laboratory **Pune**
Junior Research Fellow at National Chemical Lab), India *2008–2010*
Ab-*initio* investigations of hydrogen storage materials.
Supervisor – Prof. Sourav Pal

Pondicherry Central University **Pondicherry**
M. Sc. Dissertation, India *2006–2008*
Computational study of ring-current in aromatic molecules.
Supervisor – Prof. M.M. Balakrishna Rajan

Academic Qualifications

Computational and Materials Chemistry

Doctor of Philosophy, India *2008-2013*
National Chemical Laboratory (a premier Institute of Council of Scientific and Industrial Research (CSIR), under supervision of Prof. Sourav Pal.

Master of Science (Chemical Sciences), India *2006-2008*
Pondicherry Central University, Pondicherry. (7.34 CGPA)

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

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.*, Just Accepted Manuscript, DOI: 10.1021/acs.joc.7b02637 **(2017) (IF=4.85)**
3. **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)
4. 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)**
5. **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)
6. **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)**
7. 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)**
8. **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)**
9. **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)**

10. 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)**

11. **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)**

12. 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)**

13. **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)

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 (20), 4640- 4653. **(IF= 3.564)**

15. **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)**

16. 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)**

17. **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)**

18. **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)**

19. 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)**

20. 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)**

21. 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)**

22. **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)**

23. 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=3.582)**

24. **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)**

25. 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)**

26. 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)**

27. 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. Kim, U.H; Jun, D.W; Park, K.J; Aurbach, D; Major, D. T; Goobes, G; **Dixit, Mudit**; Leifer, N; Wang,C; Yan, P; Ahn, D; Kim, K.H; Yoon, C.S; Sun, Y. K. Pushing the limit of layered transition metal oxide cathodes for high-energy density rechargeable Li ion batteries. *(Submitted)*

Awarded Proposals

- PRACE proposal No. 2010PA3025 (2015) "Computational Design of Ni rich, Layered Oxide Based Positive Electrode Materials" was selected and awarded 300000 core hours.
- 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

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, urfaces, 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

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

Selected Invited talks and Posters

1. 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
2. Delivered an oral talk on *"Developing structure activity relationships in the dehydrogenation of alkanes on oxides"* **ACS Fall meeting (2017)**, Washington D.C. USA
3. 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
4. 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.
5. 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.
6. 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.
7. 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
8. 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
9. Presented poster on *"Underatanding the cathode materials for lithium ion batteries using first principles"*, in **IsraElectrochemistry 2014**, Tuesday, Sept. 16 2014, Technion, Israel

10 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 Ph.D. 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)

Extra-Curricular Activities

- Poems and an article published in book 'DHAWANI' NCL's first annual magazine. (2012)
- 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.

Declaration

I, the undersigned certify that to the best of my knowledge and belief, this resume correctly describes my qualifications and me.

(Mudit Dixit)

References

- **Prof. Dan T Major**,
  Associate Professor,
  Department of Chemistry,
  Bar Ilan University,
  Dan-Thomas.Major@biu.ac.il

- **3. Prof. Doron Aurbach**,
  Professor,
  Department of Chemistry,
  Bar Ilan University,
  Doron.Aurbach@biu.ac.il

- **Prof. Sourav Pal**,
  Director,
  Indian Institutes of Science Education and Research,
  s.pal@ncl.res.in, s.pal@iiserkol.ac.in

- **Prof. Boris Markovsky**,
  Professor,
  Department of Chemistry,
  Bar Ilan University,
  boris.markovsky@biu.ac.il

(more upon request)