

Gopi Krishna Phani Dathar

Postdoctoral Research Associate
Chemical Functionality Group
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Education

Kakatiya University, Warangal, INDIA	Elect. & Instr. Engineering	B.S., 2001
Louisiana Tech University, Ruston, LA	Molecular Sci. & Nanotechnology	M.S., 2006
Louisiana Tech University, Ruston, LA	Engineering (Nanotechnology)	Ph.D., 2009

Research Synopsis

Energy Storage. First principles calculations of charge/discharge processes in Li-Air Batteries; Understanding the performance of metal catalysts used in catalyzing oxygen reduction and evolution reactions; Design and development of multi-metal and metal oxide catalysts for Li-Air Batteries; First principles calculations of Li ion diffusion in materials for Lithium ion batteries; Kinetic Monte Carlo calculations of Li ion diffusion to predict charge/discharge kinetics; Thermodynamics and kinetics of hydrogen storage in transition metal doped metal hydrides.

Catalysis. Kinetics of alkane catalysis on carbon structures; Understanding Oxygen redox by Lithium on graphene and other carbon structures.

Professional Experience

2011–p	Postdoctoral Research Associate, Chemical Functionality Group, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory
2009–2011	Postdoctoral Research Associate, Department of Chemistry, University of Texas, Austin, Texas
2003–2009	Graduate Research Assistant, Institute for Micromanufacturing, Louisiana Tech University, Ruston, Louisiana

Professional and Synergistic Activities

2009–2010	Member, <i>Materials Research Society</i>
2008–p	Member, <i>Electrochemical Society</i>

Honors and Awards

2011	Selected Poster, EFRC-CST Representation in the Science for our Nation's Energy Future Summit, Washington, D.C.
2007–2008	Graduate Fellowship, Louisiana Optical Network Initiative (LONI)

Publications *List Follows CV*

Recent Invited Talks and Contributed Conference Presentations

“Theoretical Investigation of Li-Oxygen Reduction and Redox Activity of Model Carbon Structures,” G. K. P. Dathar et al., ECS Meeting, Seattle, WA, May 2012.

“Theoretical Investigation of the Li-O₂ Reduction and Evolution Reactions Catalyzed by Metal Surfaces,” G. K. P. Dathar et al, ECS Meeting, Seattle, WA, May 2012.

“Modeling Li Diffusion in Materials for Li-Ion Batteries,” G. K. P. Dathar et al, ECS Meeting, Boston, MA, Oct. 2011.

“Kinetics of Li Diffusion in Olivine Phosphates,” G. K. P. Dathar et al, Science for our Nation's Energy Future, EFRC Summit, Washington, DC, May 2011.

“Kinetics of Lithium Ion Diffusion in Olivine Phosphate (FePO₄),” G. K. P. Dathar and Graeme Henkelman, ECS Meeting, Las Vegas, NV, Oct. 2010.

Graduate and Postdoctoral Advisors:

Postdoctoral Advisors: Dr. Ye Xu, Oak Ridge National Laboratory

Dr. Graeme Henkelman, University of Texas-Austin

Graduate Advisor: Dr. Daniela Mainardi, Institute for Micromanufacturing, Louisiana Tech
University

PUBLICATIONS

Gopi Krishna Phani Dathar

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Peer-Reviewed Publications

- G. K. P. Dathar, W. A. Shelton, Y. Xu, "Trend in the Catalytic Activity of Transition Metals for the Oxygen Reduction Reaction by Lithium," *Journal of Physical Chemistry Letters* **3**, 891-895 (2012).
- G. K. P. Dathar, D. Sheppard, K. J. Stevenson, G. Henkelman, "Calculations of Li-Ion Diffusion in Olivine Phosphates," *Chemistry of Materials* **23**(17), 4032-4037 (2011).
- Y. Lu, J. B. Goodenough, G. K. P. Dathar, G. Henkelman, J. Wu, K. J. Stevenson, "Behavior of Li Guest in $\text{KNb}_5\text{O}_{13}$ Host with One-Dimensional Tunnels and Multiple Interstitial Sites," *Chemistry of Materials* **23**(13), 3210-3216 (2011).
- G. K. P. Dathar and D. S. Mainardi, "Kinetics of Hydrogen Desorption in NaAlH_4 and Ti-Containing NaAlH_4 ," *Journal of Physical Chemistry C* **114**(17), 8026-8031 (2010).
- G. K. P. Dathar and D. S. Mainardi, "Thermodynamic profiles of Ti-doped Sodium Alanates," *Journal of Physical Chemistry C* **113**(33), 15051-15057 (2009).
- G. K. P. Dathar and D. S. Mainardi, "Structure and Dynamics of Ti-Al-H Compounds in Ti Doped NaAlH_4 ," *Molecular Simulation* **34**(2), 201-210 (2008).

Peer-Reviewed Conference Proceedings

- G. K. P. Dathar and Daniela S. Mainardi, "Modeling Effects of Titanium Dopants on Hydrogen Adsorption/Desorption Kinetics by Sodium Alanates," *AIChE Conference Proceedings*, Salt Lake City, Utah, Nov. 4- 9, 2007.