

# Igor Vasiliev

## Current Research Projects

1. *Studies of the electrochemical properties of MnO<sub>2</sub> in rechargeable Zn/MnO<sub>2</sub> batteries (collaboration with Sandia National Laboratories)*. This research is focused on theoretical description of the mechanism of reversible redox reaction in rechargeable Zn/MnO<sub>2</sub> alkaline batteries.
2. *Characterization of magnetoelectric phases in nanoscale multiferroic heterostructures (collaboration with E. Fohtung)*. This research project focuses on theoretical prediction of the structural, electronic, and magnetic properties of multiferroic heterostructures at the atomic scale.

## Current Research Support

1. *Theoretical Studies of the Electrochemical Behavior of  $\gamma$ -MnO<sub>2</sub> Cathode Material in Rechargeable Zn/MnO<sub>2</sub> Batteries*, Sandia National Laboratories, 8/2017 – 9/2019, \$69,804.

## Research Personnel

- Graduate students: Birendra Ale Magar, Nirajan Paudel, Krishna Acharya

## Current Collaborations

- B. Chalamala, J. Duay, and T. N. Lambert (Sandia National Laboratories)
- E. Fohtung (New Mexico State University)

## Research Accomplishments (last 12 months)

- Journal articles:
  1. S. K. Jha and I. Vasiliev, *Vibrational Signatures of Carboxylated Graphene: A First-Principles Study*, J. Phys. Chem. C **122**, 24996–25006 (2018).
  2. I. Vasiliev, B. Ale Magar, J. Duay, T. N. Lambert, and B. Chalamala, *Ab Initio Studies of Hydrogen Ion Insertion into  $\beta$ -, R-, and  $\gamma$ -MnO<sub>2</sub> Polymorphs and the Implications for Shallow-Cycled Rechargeable Zn/MnO<sub>2</sub> Batteries*, J. Electrochem. Soc. **165**, A3517–A3524 (2018).
  3. B. Paudel, I. Vasiliev, M. Hammouri, D. Karpov, A. Chen, V. Lauter, and E. Fohtung, *Strain versus Charge Mediated Magnetoelectric Coupling Across the Magnetic Oxides/Ferroelectric Interfaces*, Nanoscale Adv. (submitted).
- One invited talk, two contributed talks (presented by students), and two poster presentations.

## Service

- College of Arts & Sciences Faculty Affairs Committee (member), Physics Curriculum Committee (chair), Engineering Physics Committee (member), Computer Committee (member), Graduate Admissions Committee (member).
- Review of research articles (JES, JPC, JPCL, MRS Comm., PSS).