

**Pabitra Choudhury**  
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## RESEARCH INTERESTS

Density functional theory (DFT) and Lattice dynamics  
Catalysis and reaction pathways  
Material synthesis and characterization (thermal, structural and chemical)

Multi-scale modeling and simulation  
Thermodynamics, structural and electronic properties of materials

## EDUCATION

- Ph.D., Chemical Engineering (GPA: 3.57) December, 2008 (expected)  
University of South Florida
- M. Tech., Chemical Engineering February, 2002  
Indian Institute of Technology, Roorkee, India
- B. Tech., Chemical Engineering April, 1999  
Indian Institute of Technology, Bombay, India

## RESEARCH EXPERIENCE

### PhD Research/Graduate Research Assistant, University of South Florida

January 2006 – Present

Thesis: Theoretical and experimental study of solid state hydrogen storage materials: complex metal boro-hydrides.  
Advisors: Prof. Venkat R. Bhethanabotla and Prof. Elias Stefanakos

Using density functional theory (DFT) and direct force constant lattice dynamics:

- Predicted material crystal structure, electronic properties and analyzed the chemical bonding of the solid state materials
- Predicted and estimated the thermodynamic stable phases, reaction pathway mechanisms of nanocatalyst doped / undoped complex materials to identify the favorable chemical reaction to maximize the yield

Using experimental techniques like thermal analysis *via.* DSC, TGA; gas sorption analysis *via.* GC, TPD, PCT and structural & chemical analysis *via.* XRD, FTIR and SEM/EDS:

- Developed the mechano-chemical procedure for the preparation of boro-hydrides/nanocatalyst doped complex composite hydrides
- Characterized the structural, surface, chemical and thermal properties of nanocatalyzed complex hydrides and investigated the structure-property relationship at nanoscale dimensions
- Study the effects of boro-hydrides/nanocatalyst doping on the reversible dehydrogenation and/or rehydrogenation characteristics (kinetics, PCT, cycle life) of complex hydrides

### M. Tech. Research, Indian Institute of Technology, Roorkee, India & Engineers India Ltd., Gurgaon, India

January 2001 – February 2002

- Developed a mathematical model to simulate the LPG sweetening process using C++ code and studied the effects of different affecting parameters

### B. Tech. Research, Indian Institute of Technology, Bombay, India

August – April 1999

- Design a process and plant for the manufacturing of 55000 tones/annum of PVC (grade 65K) using bulk polymerization.
- Designed the reactor and heat exchanger for bulk polymerization process

## PROFESSIONAL EXPERIENCE

### University of South Florida, Department of Chemical Engineering, Tampa, FL

Teaching Assistant, Mod & Analysis Engineering Systems and Transport Phenomena

### Madhav Institute of Technology & Science, Gwalior, India

March 2002 – August 2005

- Worked as a tenured lecturer in Chemical Engineering Department

- Actively involved in designing and developing the undergraduate laboratory setup
- Courses taught modeling and simulation, heat transfer, process dynamics & control, mass transfer and mechanical operations and supervised three undergraduate projects
- Design of air distribution plate for pressurized fluidized bed systems, in which a code was developed for designing of different types of distributor plate
- Worked on stochastic simulation like Monte Carlo simulation of liquid-liquid dispersion system
- Developed a new simulation procedure in C++ for the minimum area and cost target of a shell and tube heat exchangers including all the correction factors

#### **Standard Alkali Ltd., Mumbai, India**

May – August 1998

- Designed and optimized the evaporation plant of load 32% NaOH, encompassed modeling of evaporator systems, heat integration and steam utilization of the evaporation plant

### **PROFESSIONAL SKILLS**

#### **Computational Skills**

- High Level programming Languages: FORTRAN 77, C and C++
- Operating Systems: Windows, UNIX and Linux
- Advanced simulation software: Mat lab, Math CAD and Mathematica for mathematical problem solving, HYSIS and COMSOL for process simulation.
- Highly qualified to use *ab initio* software package VASP for DFT and PHONON for thermodynamics calculations of solid state materials. Proficiency in using of XCRYSDEN to get the crystal structure with atomic bonding.

#### **Laboratory Skills**

- X-ray Powder Diffraction (Philips, X'pert, Scintag), Scanning Electron Microscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDS), FTIR spectroscopy, Differential Scanning Calorimetry (DSC), Thermal Gravimetric Analysis (TGA), Pressure Concentration Temperature (PCT) apparatus, Gas Chromatography (GC), TPD Autosorb-1 for surface area analysis and chemisorptions

### **LIST OF PUBLICATIONS**

#### **Journal articles:**

1. **Choudhury, P.;** Venkat R. Bhethanabotla and Stefanakos, E., Manganese borohydride as a hydrogen storage candidate: First-principles crystal structure and thermodynamics. (manuscript under preparation).
2. **Choudhury, P.;** Chowdhury, S. and Mohanty, B., Targeting of Minimum Area and Cost of Shell-and-Tube Heat Exchangers. *Chem. Engg. Res. Des.* (manuscript submitted).
3. **Choudhury, P.;** Venkat R. Bhethanabotla and Stefanakos, E., Ni induced destabilization dynamics of crystalline zinc borohydride. *Appl. Phys. Lett.* **92**, 134101 (2008).
4. **Choudhury, P.;** Venkat R. Bhethanabotla and Stefanakos, E., Identification of a new stable phase for high capacity hydrogen storage material  $Zn(BH_4)_2$  from density functional theory and lattice dynamics. *Phys. Rev. B* **77**, 134302 (2008).
5. Chowdhury, S.; **Choudhury, P.** and Kumar, S., Monte-Carlo simulation of different dispersed liquid-liquid systems. *Indian Chem. Engr.* **47**(1), 18-24 (2005).
6. Prasad, S.; **Choudhury, P.** and Chowdhury, S., Fluidised bed systems, design of air distribution plate. *Chem. Eng. World* **38**(7), 71-73 (2003).

#### **Conference/symposium proceedings and poster presentations:**

1. **Choudhury, P.;** Bhethanabotla, V. R. and Stefanakos, E., Dehydrogenation Thermodynamics of Hydrogen Storage Material Manganese Borohydride: First-Principles Study. *AICHE Annual Meeting, Conference Proceedings*, Philadelphia, PA, United States, Nov. 16-21, (2008) (abstract submitted).
2. **Choudhury, P.;** Srinivasan, S.; Bhethanabotla, V. R. and Stefanakos, E., New Material Li-Mn-B-H System as Hydrogen Storage Candidate. *AICHE Annual Meeting, Conference Proceedings*, Philadelphia, PA, United States, Nov. 16-21, (2008) (abstract submitted).
3. **Choudhury, P.;** Srinivasan, S.; Bhethanabotla, V. R. and Stefanakos, E., Transition metal complex hydrides for vehicular application. *FLAVS Meeting*, Orlando, Florida, Mar 10-11 (2008).
4. **Choudhury, P.;** Bhethanabotla, V. R. and Stefanakos, E., *Ab-initio* calculations for Ni additives in  $Zn(BH_4)_2$ . *AICHE Annual Meeting, Conference Proceedings*, Salt lake city, Utah, United States, Nov. 4-10, (2007)
5. **Choudhury, P.;** Bhethanabotla, V. R. and Stefanakos, E., Thermodynamic stability of hydrogen storage material  $Zn(BH_4)_2$ : First principles study. *AICHE Annual Meeting, Conference Proceedings*, Salt lake city, Utah, United States, Nov. 4-10, (2007)
6. **Choudhury, P.;** Srinivasan, S.; Bhethanabotla, V. R. and Stefanakos, E., Synthesis and characterization of pure  $Zn(BH_4)_2$  single crystal. *AICHE Annual Meeting, Conference Proceedings*, Salt lake city, Utah, United States, Nov. 4-10, (2007)
7. **Choudhury, P.;** Bhethanabotla, V. R. and Stefanakos, E., Ab-initio Study of High Theoretical Hydrogen Storage Capacity Material  $Zn(BH_4)_2$ , *Florida Annual Meeting and Exposition of the American Chemical Society (FAME 2007)*, May 10-12, Orlando, Florida, USA.
8. **Choudhury, P.;** Bhethanabotla, V. R. and Stefanakos, E., First principles study of hydrogen storage material  $Zn(BH_4)_2$ . *FLAVS Meeting*, Orlando, Florida, Mar 11-13 (2007).
9. **Choudhury, P.;** Mohanty, B. and Nagpal, S., Development of mathematical modeling for the extraction of  $H_2S$  from LPG using DEA as solvent. *Proceeding of SPI - 2003*, ITBHU, Varanasi, India.