Bhaskarjyoti Borah
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Research Interests

My research interest includes design of new materials for targeted industrial applications. Currently, I am focusing on porous materials such as metal-organic frameworks that are having large surface area and hence are potential candidate for gas storage, separation of important gas mixtures, catalysis, molecular sensors and so on. The laboratory synthesis of the appropriate material for a targeted application is time consuming and difficult at times. Computational screening of large database of materials can indeed guide the experimentalist to get to the best material right away. I mainly focus on generation of databases of various relevant properties of materials and perform statistical analysis to predict the best material or the future material for a given application.

Experiences

July 2014 – Present: Assistant Professor, Physical Sciences Division, P. D. Patel Institute of Applied Sciences, Charotar University of Science and Technology, Changa, Gujarat, India

Dec 2012 – May 2014: Post – Doctoral Fellow, Chemical & Biological Engineering Department, Northwestern University, Evanston, IL, USA.

- Employing computational techniques to understand diffusion and adsorption behaviour of smaller alkanes in a large database of metal organic framework in order to screen them for natural gas storage. High-throughput computational screening of materials for targeted application. Also, involved in managing automatic backup servers and compute clusters.

April 2011 – August 2012: Scientist, Computational Research Laboratories Ltd. (Now merged with TCS), A wholly owned subsidiary by TATA Sons Ltd., Pune, India

- Mainly involved in research and development. I was responsible for various projects in the molecular simulation team. I was leading two projects :

(a) Diffusion of linear alkanes in MFI type zeolites. The project was with the collaboration with Shell Technology India, Bangalore. The main goal of the project was to understand the diffusion behaviour of long chain alkanes in the channels of silicalite using molecular simulation techniques. (b) Estimation of thermal conductivity of nanofluid with the help of molecular modelling techniques and various computational tools. The goal of the project was to understand thermal behaviour of nanofluids with various nanoparticle of various size and shape. This may eventually lead to design a better nanofluid which can act as a better coolant in engines.

Education

- Ph.D. (2011) − Computational Condensed Matter Physics, Indian Institute of Science, Bangalore-560012, India
- M.Sc. (2003) − Physics, Indian Institute of Technology Guwahati, Guwahati - 781039, Assam, India [CPI 7.9/10, 3rd rank]
- B.Sc. (2001) − Physics(Honours), Chemistry and Mathematics, Gauhati University, Guwahati – 781001, Assam, India [First class 2nd with distinction; 72% in honours]

Sponsored Research:

- DST-SERB sponsored project (Sept 2016 – August 2019) of amount 39.7 lacs. The project deals with separation of hydrocarbon isomers as per requirement of petrochemical industries.

Patents

- *Metal Organic Frameworks with Ultrahigh Surface Areas*; Omar K. Farha, Joseph T. Hupp, Christopher E. Wilmer, Ibrahim Eryazici, Randall Q. Snurr, Diego A. Gomez-Guzldron, and **Bhaskarjyoti Borah;** US Patent Application number PCT/US2013/046254

Scientific Publications

- Viral A Solanki and ***Bhaskarjyoti Borah****, Exploring the Potentials of Metal–Organic Frameworks as Adsorbents and Membranes for Separation of Hexane Isomers, *J. Phys. Chem. C*, 123, 17808-17822, 2019

- ***Bhaskarjyoti Borah***, Hongda Zhang, Randall Q. Snurr; Diffusion of methane and other alkanes in metal-organic frameworks for natural gas storage, *Chem. Eng. Sci*., 124, 135-143, 2015

- Diego A. Gomez-Gualdron, Oleksii V. Gutov, Vaiva Krungleviciute, ***Bhaskarjyoti Borah***, Joseph E. Mondloch, Joseph T. Hupp, Taner Yildirim, Omar K. Farha, and Randall Q. Snurr; Computational Design of Metal–Organic Frameworks Based on Stable Zirconium Building Units for Storage and Delivery of Methane, *Chem. Mater.*, 26, 5632 – 5639, 2014

- Rajappa, Chitra; Krause, C.; ***Borah, B.J.***; Adem, Z.; Galvosas, P.; Kärger, J.; Subramanian, Y. : "Diffusion of pentane isomers in faujasite-type zeolites : NMR and molecular dynamics study", *Microporous and Mesoporous Materials*, 171, 58-64, 2013.

- ***Bhaskar J. Borah***, Prabal Maiti, Charusita Chakravarty, and Yashonath Subramanian; Transport in Nanoporous Zeolites : Relationships between Sorbate Size, Entropy, and Diffusivity, *J. Chem. Phys*., 136, 174510, 2012 (Selected for Virtual Journal of Nanoscale Science & Technology, May 21, 2012)

- ***Bhaskar J. Borah*** and S. Yashonath; Ions in water: Role of attractive interaction in size dependent diffusivity maximum., *J. Chem. Phys*., 133, 114504, 2010 (Selected for Virtual Journal of Biological Physics Research, October 1, 2010 issue)

- ***Bhaskar J. Borah***, Herve Jobic and Yashonath Subramanian; Levitation Effect in Zeolites : Quasi-elastic neutron scattering and molecular dynamics study of pentane isomers in zeolite NaY, *J. Chem. Phys*., 132, 144507, 2010.

- Deroche, G. Maurin, ***B. J. Borah***, S. Yashonath and H. Jobic; Diffusion of Pure CH4 and Its Binary Mixture with CO2 in Faujasite NaY: A Combination of Neutron Scattering Experiments and Molecular Dynamics Simulations, *J. Phys. Chem C*, 114, 5027, 2010.

- Herve Jobic, ***Bhaskar J. Borah*** and Subramanian Yashonath; Neutron Scattering and Molecular Dynamics Evidence for Levitation Effect in Nanopores., *J. Phys. Chem B*, 113, 12635, 2009.

- F. G. Pazzona, ***B. J. Borah***, P. Demontis, G. B. Sufriti and S. Yashonath; A Comparative Molecular Dynamics Simulation Study of Diffusion of n-decane and 3-methyl pentane in Y Zeolite., *J. Chem. Sci.*, 121, 921, 2009.