Brijith Thomas

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Profile

The primary focus of my research is in the field of application of solid state NMR to solve the problems associated with the energy crisis. During my Ph.D. (with Prof. Huub de Groot) at Ledien University, Netherlands, we developed a novel methodology to solve the supra molecular structure of the molecule used in artifical photosynthesis using solid state NMR, Electron Nano Crystallography and Quantum Mechanical modelling. The theme of Huub's group was to study about the interaction between light and materials in the case of natural photosynthesis and how it could be successfully mimicked for artificial photosynthesis. The work was a part of 'bio solar cell consortium', which is one of the first artificial solar fuel cell projects in Europe. During my stay at Ames Laboratory, Iowa, USA (with Dr. Aaron J. Rossini), my focus was to use the state of the art Dynamic Nuclear Polarisation (DNP) - SSNMR to understand the mechanism of an industrially relevant heterogeneous catalyst. Currently at Weizmann Institute of Science, Rehovot, Israel (with Dr. Michal Leskes), I am involved in the development of DNP methodology to understand the solid electrolyte used in the battery and about how the disorder of a system can affect the DNP mechanism. And in the future I want to use solid state NMR with other complementary techniques to do novel chemistry associated with energy crisis.

Summary of Skills

Nine years hands on experience on various projects using SSNMR, DNP-SSNMR, Electron Paramagnetic Resonance, PXRD, Simpson, Spinevolution,Easy Spin, Matlab and DFT calculations. This includes designing and successful implementation of various projects. Demonstrated teamwork skills by working as a member of an interdisciplinary team spread across different countries.

The Ph.D. project was a part of the 'Biosolar Cell' consortium of the Dutch government and 'Euro Solar Fuel Cell' consortium of the European union. The interactive environment in the consortium and working together with different groups helped me to develop interpersonal skills to associate with diverse groups to address a challenging problem and help (or guide) other associated fields from the framework of solid state NMR.

Supervised undergraduate students with their Bachelors and Masters project.

Served as the representative to the postdoctoral Association at Iowa State University, Ames, Iowa.

Educational Qualifications

2019 – - **Postdoctoral Deans Fellow,** Advisor: *Dr. Michal Leskes*
Weizmann Institute of Science, Rehovot, Israel
(https://www.weizmann.ac.il/)
Research: Methodological development of Metal Ion Dynamic Nuclear Polarisation (MIDNP) for solid state electrolyte

2017 – 2019 **Postdoctoral Research Associate**, Advisor: *Dr. Aaron J. Rossini*
Ames Laboratory, Iowa, USA
(https://www.ameslab.gov/)
Research: DNP - SSNMR to study the mechanisms of industrially important heterogeneous catalysts

2012 – 2016 **Ph.D. in Chemistry**, Advisor: *Prof. Huub J. M. de Groot*
Leiden University, Leiden, Netherlands
(https://www.universiteitleiden.nl/)
Research: Towards artificial photosynthesis – Resolving supramolecular packing of artificial antenna chromophores through a hybrid approach-ISBN: 9789462955189

2009 – 2011 **Masters in Chemistry**, Advisor: *Prof. R. Karvembu*
National Institute of Technology Tiruchirappalli, Tamil Nadu
(https://www.nitt.edu/)
Research: Copper on Boehmite: Efficient nano catalyst for the synthesis of beta ketoenamines, Obtained 9.34 CGPA

2006 – 2009 **Bachelors in Chemistry**, obtained 93.4 % in Chemistry
Mahatma Gandhi University, Kottayam, Kerala
(https://www.mgu.ac.in/)

Peer-reviewed Scientific Publications

1. Endogenous dynamic nuclear polarization for sensitivity enhancement in solid state NMR of electrode materials.
   Adi Harchol, Guy Reuveni, Vitallii Ri, **Brijith Thomas**, Raanan Carmieli, Rolfe H. Herber, Chunjoong Kim, Michal Leskes.
   J. Phys. Chem. C. 13, 7082-7090 (2020). [IF: 4.1]
2. Synthesis of interface driven tunable band gap metal oxides.
   Boyce S. Chang, Andrew Martin, **Brijith Thomas**, Ang Li, Rick W. Dorn, Jinlong Gong, Aaron J. Rossini, Martin M. Thuo.
   ACS Materials Lett. 2, 1211-1217 (2020).
3. B-MWW zeolite: the case against single-site catalysts.
   Natalie R. Altvater, Rick W. Dorn, Melissa C Cendejas, William P. Mc Dermott, **Brijith Thomas**, Aaron J. Rossini, Ive Hermans.

Angew. Chem. Int. Ed. 132, 6608-6612 (2020). [IF: 12.9]

4 Ambient synthesis of nanomaterials by insitu heterogenous metal/ligand reactions.

Boyce S Chang, **Brijith Thomas**, Jiahao Chen, Ian D. Tevis, Paul Karanja, Simge Sinar, Amrit Venkatesh, Aaron J. Rossini, Martin M. Thuo.

Nanoscale 29, 14060-14069 (2019). [IF: 6.8]

5 Synthesis and characterization of silica supported boron oxide catalysts for the oxidative dehydrogenation of propane.
Alyssa M Love, Melissa C Cendejas, **Brijith Thomas**, William P. Mc Dermott, Pajean Uchupalanun, Catherine Kruszynski, Samuel P Burt, Theodore Agbi, Aaron J. Rossini, Ive Hermans.

J. Phys. Chem. C. 44, 27000-27011 (2019). [IF: 4.1]

6. Probing the oxidative transformation of boron nitride catalysts under oxidative dehydrogenation conditions.
Brijith Thomas,# Alyssa M. Love,# Sarah E. Specht, Michael P. Hanrahan, Juan M. Venegas, Samuel P. Burt, Joseph T. Grant, Melissa C. Cendejas, William P. McDermott, Aaron J. Rossini, Ive Hermans. # indicates equal contribution.

J. Am. Chem. Soc. 1, 182-190 (2019). [IF : 14.6]

7. A molecular level approach to elucidate the supramolecular packing of light harvesting antenna systems.

Brijith Thomas, Rajeev K. Dubey, Max Clabbers, Karthick Babu Sai Sankar Gupta, Wolter F. Jager, Jan Pieter Abrahams, Huub J. M. de Groot.

Chem. Eur. J. 24, 14989–14993 (2018). [IF: 4.8]

8. Determination of controlled self-assembly of fused NDI-salphen by homology modeling with hybrid NMR and TEM.

Brijith Thomas, Jeroen Rombouts, Karthick Babu Sai Sankar Gupta, Francesco Buda, Koop Lammertsma, Romano Orru, Huub J. M. de Groot.

Chem. Eur. J. 23, 9346–9351 (2017). [IF: 4.8]

9 A hybrid solid state NMR electron microscopy structure determination protocol for engineering advanced para-crystaline optical materials.

Brijith Thomas, Rajeev K. Dubey, Max Clabbers, Karthick Babu Sai Sankar Gupta, Wolter F. Jager, Jan Pieter Abrahams, Huub J. M. de Groot.

Chem. Eur. J. 23, 3280–3284 (2017). [IF: 4.8]

10 Molecular catalytic assemblies for electrodriven water splitting.

Khurram Saleem Joya, Jose L. Vallés-Pardo, Yasir F. Joya, Thomas Eisenmayer, **Brijith Thomas**, Francesco Buda, Huub J. M. de Groot.

ChemPlusChem 78, 35–47 (2013). [IF: 2.7]

11 Cu/AlO(OH)-catalyzed formation of beta-enamino ketones/esters under solvent, ligand and base free conditions - experimental and computational studies.

Sundaram Ganesh Babu, **Brijith Thomas**, Abdulrahiman Nijamudheen, Ayan Datta, Ramasamy Karvembu.
Catal. Sci. Technol. 2, 1872–1878 (2012). [Published during Masters] [IF: 5.7]

Scientific Publications under Preparation

12. Probing the effect on the Fe and Gd dopant on the signal enhancement of LLZO.
    Brijith Thomas, Michal Leskes.
13. Solid state- NMR assisted structure determination of coordination polymers.
    Brijith Thomas, Boyce S. Chang, Aaron J. Rossini, Martin M. Thuo.
14. Influence of molecular structure of lithium calcium silicate on the metal ion DNP.
    Brijith Thomas, Michal Leskes.

Conferences and Presentations

2018 Rocky Mountain Conference, Colorado, USA, 2018

2016 Developments and Applications of Solid State NMR to Materials Science, Chemistry and Engineering Conference, Bulgaria, 2016

2016 International Conference and Exhibition on Materials Chemistry, Valencia, Spain - oral presentation

2015 NMRDG Meeting, Netherlands

2015 ISMAR Conference, Shanghai, China - oral presentation

2015 The 9^{th} Alpine Conference on Solid State NMR, Chamonix Mont-Blanc, France

2015 The 11^{th} Euromar, Prague, Czech Republic

2014 Solar Fuel Cell Meeting, Passau, Germany

2014 SMARTER4 Conference, Durham University, UK

2014 The 55^{th} Experimental Nuclear Magnetic Resonance Conference, Boston, Massachusetts

2013 The 8^{th} Alpine Conference on Solid State NMR, Chamonix Mont-Blanc, France

2013 EuroSolarFuel Meeting, Torun, Poland

2013 The 9^{th} Euromar, Hersonissos, Crete

2012 First EuroSolarFuels conference Glasgow, UK - oral presentation

Project Work

1. **Theoretical investigation into the rearrangement of orthocarborane to metacarborane**

   Guide: Prof. K. L. Sebastian, Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bengaluru, India.

I received fellowship from Indian academy of sciences to carry out the project. Summer fellowship project was to find the rearrangement mechanism in carborane using Gaussain 09 software.

2. **Copper on Boehmite: Efficient nano catalyst for the synthesis of beta ketoenamines** (Master's Thesis)

   Guide: Prof. R. Karvembu, Department of Chemistry, National Institute of Technology Tiruchirappalli, Tamil Nadu, India

   Cu/AlO(OH) has been found to be an efficient catalyst for the formation of β -enamino ketones/esters under solvent, ligand and base free conditions.The catalyst Cu/AlO(OH) is prepared from $CuCl_2 \cdot 2H_2O$, pluronic P123 and Al(O-sec-Bu)$_3$. The prepared catalyst is characterized by HR-TEM, SEM-EDX, XPS and FT-IR spectra. The β-ketoenamine is prepared using Cu/AlO(OH) as catalyst under mild and environmentally benign conditions. The reaction conditions are optimized with different catalyst amounts and temperatures using an acetylacetone and aniline system as a model. The scope of the reaction is extended to different types of diketones and amines. Solvent, ligand and base free and room temperature conditions make the reaction interesting from both an economic and environmental point of view. A mechanism is proposed on the basis of DFT calculations.

3. **Towards artificial photosynthesis – Resolving supramolecular packing of artificial antenna chromophores through a hybrid approach** (Ph.D. Thesis - pdf available online: http://hdl.handle.net/1887/44146)

   Guide: Prof. Huub de Groot, Leiden Institute of Chemistry, Leiden University, Netherlands.

   Photosynthesis is a highly cross linked process. However, we can distinguish a set of fundamental building blocks like chlorophylls, which interact to form photosystem, which performs the complex function of water splitting. The key challenge in artificial photosynthesis is to learn how to design systems that can adapt and optimize their topologies in line with self-assembly of natural photosystem. In this thesis I combine different techniques of cross polarization Magic angle spinning Nuclear Magnetic Resonance and Transmission Electron Microscopy (TEM) with simulation and modeling, to resolve the global packing of molecules which are potential candidates for efficient solar fuel cell devices. This thesis focuses on the packing analysis of three-dimensional structures, which are heterogeneous in nature. I demonstrate a new and general structure determination approach that, in combination with first-principles quantum chemical calculations, establishes the structures of molecularly ordered antenna complexes that lack long-range 3D atomic crystalline order. This is possible despite the absence of a priori information on the space group or atomic coordinates.In summary, a novel methodology to resolve the structure of chromophore antenna from a structural background with static and dynamic heterogeneity that strongly limits the diffraction response is shown. Furthermore, I anticipate that the insights into packing of the antenna are key to the design of the organic solar fuel cell device in the future.

4. **Characterization of heterogeneous catalysts using dynamic nuclear polarization (DNP) ^{11}B NMR and ^{69}Ga NMR**

   Hexagonal boron nitride (h-BN) and boron nitride nanotubes (BNNT) were recently reported as highly selective catalysts for the oxidative dehydrogenation (ODH) of alkanes to olefins in the gas phase. Previous studies revealed a substantial increase in surface oxygen content after exposure to ODH conditions (heating to 500 °C under a flow of alkane and oxygen); however, the complexity of these materials has thus far precluded an in-depth understanding of the oxygenated surface species. In this contribution, we combine advanced NMR spectroscopy experiments with scanning electron microscopy and soft X-ray absorption spectroscopy to characterize the molecular structure of the oxygen functionalized phase that arises on h-BN and BNNT following catalytic testing for ODH of propane. The pristine BN materials are readily oxidized and hydrolyzed under ODH reaction conditions to yield a phase consisting of three-coordinate boron sites with variable numbers of hydroxyl and bridging oxide groups which is denoted $B(OH)_xO_{3-x}$ (where x = 0–3). Evidence for this robust oxide phase revises previous literature hypotheses of hydroxylated BN edges as the active component on h-BN.

5. **Probing the effect on the Fe and Gd dopant on the signal enhancement of LLZO (ongoing)**

   Influence of Fe and Gd dopant on the DNP sweep profile of LLZO is studied. The mechanism observed was Solid Effect for the ^{6}Li and ^{7}Li Gd doped LLZO at low concentration. In the case of Fe doped LLZO the asymmetric dopant site leads to a different mechanism. This study paves way to choose the dopant for the solid electrolytes and using it to understand the mechanism of lithium transport.

Teaching Experience

Teaching Assistant — Assisted in the solid state NMR course at Leiden University, Netherlands.

Research Assistant — Worked as undergraduate course assistant in Leiden University. Carried out examination and evaluation duties assigned by Leiden Institute of Chemistry, Leiden University, Netherlands.

References

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