Jissy A. K.

PhD, Computational Chemistry

Current Position

Jan 2016 -present **Postdoctoral Researcher** at Karlsruhe Institute of Technology, Karlsruhe, Germany

Advisor Prof. Dr. Marcus Elstner

Publications

13. Scharf, P.; Biswarup J.; **Jissy, A. K.**; Waller, M. P.; Müller, J. "Sequence-dependent duplex stabilization upon formation of a metal-mediated base pair", Chem. A Eur. J, **2015** (accepted).
12. **Jissy, A. K.**; Datta, A. "Design and Applications of Noncanonical DNA Base Pairs" *J. Phys. Chem. Lett. (Perspective),* **2014**, *5*, 154.
11. **Jissy, A. K.**; Sanjay, K. M.; Datta, A. "Reactivity of Gemanones: Far Apart from Ketones - A Computational Study" *RSC Adv.,* **2013**, *3*, 24321.
10. **Jissy, A. K.**; Datta, A. "Can Arsenates Replace Phosphates in Nature? A Computational Study" *J. Phys. Chem. B,* **2013**, *117*, 8340.
9. **Jissy, A. K.**; Datta, A. "What Stabilizes the LinPn Inorganic Double Helices?" *J. Phys. Chem. Lett.,* **2013**, *4*, 1018.
8. **Jissy, A. K.**; Sukanya, K.; Datta, A. "Molecular Switching Behavior in Isosteric DNA Base Pairs" *Chem. Phys. Chem.,* **2013**, *14*, 1219.
7. **Jissy, A. K.**; Datta, A. "Effect of External Electric Field on H-Bonding and π-Stacking Interactions in Guanine Aggregates" *Chem. Phys. Chem.,* **2012**, *13*, 4163.
6. **Jissy, A. K.**; Ashik, U. P. M.; Datta, A. "Nucleic Acid G-quartets: Insights into Diverse Patterns and Optical Properties" *J. Phys. Chem. C,* **2011**, *115*, 12530. **[Selected for Cover Page of the J. Phys. Chem. C, June 30 issue]***
5. **Jissy, A. K.**; Ramana, J. H. V.; Datta, A. "π-stacking Interactions between G-quartets and Circulenes: A Computational Study" *J. Chem. Sci.* **2011**, *123*, 891. [**Invited contribution in the journal's Special Issue celebrating the International Year of Chemistry (IYC) 2011]**
4. **Jissy, A. K.**; Datta, A. "Isophlorin Derivatives: Structures and Materials for n-Channel Organic Semiconductors" as a **chapter in "Atomic and Molecular Nonlinear Optics: Theory, Experiment and Computation", IOS Press** 94-109, **2011**.
3. L. Rajith; **Jissy, A. K.**; K. G. Kumar; Datta, A. "A Mechanistic Study for the Facile Oxidation of Trimethoprim on Manganese Porphyrin Incorporated Glassy Carbon Electrode" *J. Phys. Chem. C,* **2011**, *115*, 21858.
2. **Jissy, A. K.**; Datta, A. "Designing Molecular Switches Based on DNA-Base Mispairing" *J. Phys. Chem. B,* **2010**, *114*, 15311.

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1. **Jissy, A. K.**; Datta, A. "Isophlorin Derivatives: Structures and Materials for n-Channel Organic Semiconductors" *J. Comput. Meth. Sci. Eng.* **2010**, *10*, 189.

**Our theoretical prediction of G4-K^+ complexes to be the most effective molecular system for realistic optical birefringence applications was experimentally verified by Das et al. They reported supramolecular hydrogels prepared by the potassium-ion-mediated self organization of guanosine and 8-bromoguanosine. These guanosine-based supramolecular structures exhibit strong birefringence (0.07 - 0.1) in the presence of dyes. (Das, R. N.; Kumar, Y. P.; Pagoti, S.; Patil, A. J.; Dash, J. Diffusion and Birefringence of Bioactive Dyes in a Supramolecular Guanosine Hydrogel. Chem. Eur. J. 2012, 18, 6008-6014.)*

Research Interests

Keywords Computational Biochemistry, Density Functional Theory, Tight-binding Density Functional Theory, Non-covalent interactions, cooperativity, Multi-scale Modeling, Graph Theory, Fragmentation QM/MM methods, Machine Learning, Structure and electronic properties of DNA and proteins, Biomolecular nanostructures, Protein-DNA binding, DNA mispairing, Metal-mediated base pairing, Artificial nucleobases.

Current Research Interests

- Enzyme catalysis
- Quantum mechanical investigation of biomolecular reactions
- Quantum mechanical and QM/MM DNA modeling, DFT studies of metal-mediated base-pairs, artificial base pairs
- Quantum mechanical treatment of large biomolecules by fragmentation adaptive QM/MM methods
- Coupling adaptive QM/MM methods with molecular dynamics
- Molecular machines
- Molecular modeling of novel clusters

Technical skills

- Experienced in DFT, DFT-D, TD-DFT, Energy Decomposition Analysis (EDA).
- Experienced user of : GROMACS, AutoDock, Gaussian, ADF, Turbomole, Gabedit, Hyerchem, NBO.
- Visualization and analysis of non-covalent interactions: AIM, NCIPLOT.
- Programming Languages: Java, R, Groovy.
- Experienced user of Neo4j, Cypher.
- Plotting: Plotly, Gliffy, Origin, Xmgrace.
- Visualization of structures and molecules: GaussView, Molden, Mercury, VMD, Chimera, ADF-view, Pymol, Rasmol.
- Use of parallel clusters.
- Experienced in all main Operating Systems - Unix/Linux, Windows, OS X.

Research Experience

Jan 2016 - **Postdoctoral Researcher** at Karlsruhe Institute of Technology, Karlsruhe

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Advisor Prof. Dr. Marcus Elstner

Jul 2014 - Jun 2015 **Postdoctoral Researcher** at Westfälische Wilhelms-Universität Münster

Advisor Mark Waller, Ph.D

Jan 2010 - Aug 2013 **Doctoral Research Fellow** at Indian Institute of Science Education and Research, Trivandrum

Advisor Prof. Ayan Datta

Topic Computational Studies on Derivatives of DNA Base-Pairs and Other Biomolecules

Nov 2006 - Jan 2007 **Research Assistant** at Laboratoire de Chimie Organique, Universite Pierre et Marie Curie, France

Advisor Prof. Max Malacria

Topic Stereoselective Route for the Synthesis of Polyhydroxy Piperidines

Jan 2006 - May 2006 **Student Researcher** at Indian Institute of Technology, Roorkee

Advisor Prof. R.K. Peddinti

Topic Tandem Oxidative Acetalization (Intramolecular) Diels-Alder Reactions of Guaiacol and Methyl Iso-vanillate

May 2005 - Jul 2005 **Visiting Summer Research Student** at Tata Institute of Fundamental Research, Mumbai

Advisor Prof. N. Periasamy

Topic Synthesis and Spectroscopic Studies of Trihydroxy Benzene Based Xanthene Dyes

Teaching Experience

2015 Teaching Assistant, Computer application - University of Muenster.

2012 Teaching Assistant, Computational Chemistry - IISER-TVM.

2010 Teaching Assistant, Kinetics and Mechanism - IISER-TVM.

2010 Student Supervisor in Chemistry Laboratory, IISER-TVM.

2010-2013 Summer and Visiting Student Supervisor.

Awards and Fellowships

2011 Financial Grant from Department of Science and Technology **(DST)**, India to present work in ESF Research Conference on "Charge Transfer in Biosystems", Austria.

2009 National Junior Research Fellowship **(JRF)** for Ph.D program by University Grants Commission **(UGC)**, India.

2006 Qualified National Graduate Aptitude Test in Engineering **(GATE)**

2005 Summer Research Fellowship for Visiting Students Research Programme **(VSRP)**, - Tata Institute of Fundamental Research **(TIFR)**, Mumbai.

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2004 Qualified Joint admission Test for Masters **(JAM)**, **IIT**.

2004 *Durga Devi memorial Prize* for **First Position**, B.Sc. Chemistry, **Delhi University**.

Poster Presentations

Feb, 2013 Electronic Structure and Dynamics of Molecules and Clusters, Indian Association for the Cultivation of Science, Kolkata, India.

Mar, 2012 Sixth RNA Group Meet, IISc Bangalore, India.

Jul, 2011 ESF Research Conference, Obergurgl, Austria.

Dec, 2011 Inter IISER Chemistry Meet, IISER-TVM.

Mar, 2011 IISER Chemistry Group Meeting, IISER-TVM.

Mar, 2011 Biomolecular Simulation Algorithm and Application, JNU, Delhi.

Dec, 2010 Theoretical Chemistry Symposium, IIT Kanpur.

Jun, 2010 Performance Enhancement on Multi-Core Processors and GPUs at C-DAC

Apr, 2010 Emergent Properties and Novel Behaviour at the Nanoscale, JNCASR Bangalore, India. Bangalore, India.

Conferences and Workshops

May, 2015 6th Münster Symposium on Cooperative Effects in Chemistry, Münster, Germany.

Mar, 2015 The 2015 CMTC Workshop on Computing Free Energy Across Disciplines: From Method Development to Applications, Münster, Germany.

Jan, 2015 Münster-Twente-Minisymposium on Multiscale Theory and Computation, Münster, Germany.

Feb, 2013 International Conference on "Electronic Structure and Dynamics of Molecules and Clusters", Indian Association for the Cultivation of Science, Kolkata, India.

Mar, 2012 Sixth RNA Group Meet, IISc Bangalore, India.

Dec, 2011 Inter IISER Chemistry Meet 2011, IISER-TVM, Trivandrum, India.

Jul, 2011 ESF Research Conference on Charge Transfer in Biosystems, Obergurgl, Innsbruck, Austria.

Mar, 2011 Conference on Biomolecular Simulation Algorithm and Application, JNU, Delhi, India.

Dec, 2010 Theoretical Chemistry Symposium, IIT Kanpur, India.

Jul, 2010 5^{th} mid-year CRSI Symposium in Chemistry, NIIST, Trivandrum, India.

Jun, 2010 Performance Enhancement on Multi-Core Processors and GPUs, C-DAC Bangalore, India.

Apr, 2010 Emergent Properties and Novel Behaviour at the Nanoscale, JNCASR Bangalore, India.

Education

PhD (2010 - 2013) Computational Biochemistry, **Indian Institute of Science Education and Research (IISER), Thiruvananthapuram**

Advisor Prof. Ayan Datta

Thesis Computational Studies on Derivatives of DNA Base-Pairs and Other Biomolecules

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MSc (2004 - 2006) Chemistry (Organic Specialization), **Indian Institute of Technology (IIT), Roorkee**

Advisor Prof. R.K. Peddinti

Thesis Tandem Oxidative Acetalization (Intramolecular) Diels-Alder Reactions of Guaiacol and Methyl Iso-vanillate

BSc (2001 - 2004) Chemistry (Honors), **Delhi University, Delhi.** ***First Rank***

Personal Details

Date of Birth 09.30.1983

Sex Female

Languages English (fluent), Hindi (fluent), Malayalam (mother tongue), French (beginner), German (beginner)

Nationality Indian

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