Oinam Romesh Meitei

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Education

Aug. 2015 – Sep. 2018 **Ph.D. Chemistry (Dr. rer. nat.)**
Friedrich-Alexander University, Erlangen, Germany
Thesis: *Development of a molecular fragmentation method for the description of intra-molecular interactions in large molecules.*
Advisor: Dr. Andreas Hesselmann

July 2013 – May 2015 **M.Sc. Chemistry**
Visvesvaraya National Institute of Technology, Nagpur, India
Thesis: *PCM Vs C-PCM on the vertical excitation of oligoacenes.*
Advisor: Dr. Sujit Kumar Ghosh

June 2010 – May 2013 **B.Sc. Chemistry**
Madras Christian College, University of Madras, Chennai, India
Project: *Electrochemical & theoretical study on the adsorption characteristic of 4-hydroxyquinazoline & Lumazine as corrosion inhibitor for mild stell.*
Advisor: Dr. Paul Wilson

Fellowship & Grant

May 2013 **Summer Research Fellowship**, Indian Academy of Science, Bangalore, India

Sep. 2012 **Start College Project Grant**, Department of Biotechnology, Govt. of India

Professional Experience

Mar. 2019 – Present **Postdoctoral Associate**, Virginia Tech, Blacksburg, USA
Advisor: Dr. Nicholas J. Mayhall
- *Developed a gate-free hybrid quantum classical variational algorithm for molecular simulations on near-term quantum computers.*
- *Developed a combined Fock-space CI and pair-density functional theory approach.*
- *Developed a perturbative spin-orbit coupling treatment for Fock-space CI methods.*

Aug. 2015 – Dec. 2018 **Research Associate**, University of Erlangen-Nuremberg, Erlangen, Germany
Advisor: Dr. Andreas Hesselmann
- *Developed low-order scaling incremental molecular fragmentation method for electron-correlation wavefunction methods.*
- *Derived molecular energies, nuclear gradients and molecular properties.*
- *Developed methodologies for accurate description of intramolecular interactions in large molecules, including a quantum embedding approach.*

Summer Research/School

May – July 2014/2015 **Summer Research Fellow**, National Chemical Laboratory, Pune, India
Advisor: Dr. Sourav Pal
- *Studied the charge transfer state and the influence of intermolecular interaction in small molecule organic semiconductor using TD-DFT.*

Sept. 2017 **Summer School**, 16^{th} European summer school in quantum chemistry, Sicily, Italy

Publications

11. Gate-free state preparation for fast variational quantum eigensolver simulations
O. R. Meitei, B. T. Gard, G. S. Barron, D. P. Pappas, S. E. Economou, E. Barnes, N. J. Mayhall
arXiv:2008.04302 [quant-ph]

10. Spin-Orbit Matrix Elements for a Combined Spin-Flip and IP/EA approach
O. R. Meitei, S. E. Houck and N. J. Mayhall
J. Chem. Theory Comput, 16, 3597, 2020

9. Geometry optimisations with the incremental fragmentation method
O. R. Meitei and A. Hesselmann
J. Theor. Comput. Chem., 17, 1850037, 2018

8. Intermolecular dispersion energies from coupled exact-exchange Kohn-Sham excitation energies and vectors
A. Hesselmann and **O. R. Meitei**
Comput. Theor. Chem., 1129, 57, 2018

7. Intramolecular interactions in sterically crowded hydrocarbon molecules
O. R. Meitei and A. Hesselmann
J. Comput. Chem, 38, 2500, 2017

6. On the stability of cyclophanes derivates using a molecular fragmentation method
O. R. Meitei and A. Hesselmann
Chem. Phys. Chem., 17, 3863, 2016 **Featured as journal cover**

5. Molecular energies from an incremental fragmentation method
O. R. Meitei, A. Hesselmann
J. Chem. Phys., 144, 094109, 2016

4. Conformation controlled turn on- turn off phosphorescence in metal free biluminophore: Thriving the paradox that exists for organic compounds
R. Joshi, **O. R. Meitei**, M. Jadhao, H. Kumar and S. K. Ghosh
Phys. Chem. Chem. Phys., 18, 27910, 2016

3. ESIPT Reaction of Potential Bioactive Heterocyclic Schiff Base: Atomic Visualization Coupled with In vitro Spectroscopy
M. Jadhao, **O. R. Meitei**, R. Joshi, H. Kumar, C. Das and S. K. Ghosh
Journal of Photochemistry and Photobiology A: Chemistry, 326, 41, 2016

2. Design, synthesis and proticity inclined conformational modulation in a highly fluorescent bichromophoric naphthalimide derivative: Hind directed from RICT perspective
R. Joshi, **O. R. Meitei**, H. Kumar, M. Jadhao and S. K. Ghosh
J. Phys. Chem. A., 120, 1000, 2016

1. Surfactant induced aggregationdisaggregation of photodynamic active chlorin e6 and its relevant interaction with DNA alkylating quinone in a biomimic micellar microenvironment
M. Jadhao, P. Ahirkar, H. Kumar, R. Joshi, **O. R. Meitei** and S. K. Ghosh
RSC Advances, 5, 81449, 2015

Oral Presentations

6. Gate-free state preparation for fast variational quantum eigensolver simulations
Contributed Talk, *Quantum week of fun (QCxQC), Cambridge Quantum Computing (Virtual), Sept. 2020*

5. Spin-orbit matrix elements for a combined spin-flip and IP/EA approach
Contributed Talk *(Cancelled due to COVID-19), ACS Spring 2020 National Meeting & Expo, Philadelphia, USA, Mar. 2020*

4. Molecular properties from the incremental fragmentation method
Contributed Talk, *Third summer school of the DFG SPP, Hamburg, Germany, July 2018*

3. An incremental molecular fragmentation method
Seminar Talk, *Group of Prof. Andreas Goerling, University of Erlangen-Nuremberg, Germany, Jan. 2018*

2. Efficient geometry optimization of extended molecules using an incremental fragmentation method
Contributed Talk, *Second summer school of the DFG SPP, Rostock, Germany, July 2017*

1. On the stability of cyclophanes derivates using molecular fragmentation method
Contributed Talk, *First summer school of the DFG SPP, Bremen, Germany, May 2016*

Poster Presentations

8. Optimal control in variational quantum simulation for molecules
Virtual Conference on Theoretical Chemistry, Virtual, July 2020

7. Spin-orbit matrix elements for a combined spin-flip and IP/EA approach
60^{th} Sanibel Symposium, St. Simons Island, USA, Feb. 2020

6. A practical approach to intramolecular interactions via molecular fragmentation
54^{th} Symposium on theoretical chemistry, Halle(Saale), Germany, Sept. 2018

5. Molecular properties from an incremental fragmentation method
   Second workshop of the DFG SPP, Cologne, Germany, Oct. 2016
4. Molecular properties from an incremental fragmentation method
   52th Symposium on theoretical chemistry, Bochum, Germany, Sept. 2016
3. On the stability of cyclophanes derivates using molecular fragmentation method
   CECAM workshop: Density and response density based models for intermolecular interactions in molecular assemblies and in solids, Nancy, France, June 2016
2. Conformational energies from a systematic molecular fragmentation
   First workshop of the DFG SPP, Goettingen, Germany, Oct. 2015
1. A DFT approach to reactivity of diazoaminobenzene
   Symposium on Dynamics of Complex Chemicals and Biological Systems, Kanpur, India, Feb. 2014

Software Development

CtrlQ Tool for simulating transmon qubit device for gate-free state preparation in variational quantum eigensolver. Written in Python and C++.
https://github.com/oimeitei/ctrq

Fragpy Massively parallel Python library for geometry optimization using molecular fragmentation method.
https://github.com/oimeitei/fragpy

Molepy Python based quantum chemistry program with the computationally demanding modules in C++ (experimental state).
https://github.com/oimeitei/molepy

Skills

Programming Languages:
Python, C/C++, Fortran

Running packages:
OpenMolcas, Pyscf, Dalton, Molpro, PSI4, Turbomole, QChem, Gaussian

Others

Languages Manipuri (native), English (fluent), Hindi (Conversational), German (beginner)

Interests Trekking, Via Ferrata, Skiing, Kayaking, Folk Music