SHIVANAND KUMAR VEESAM

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PROFILE

PhD candidate in chemical engineering trained in multiscale computational thermodynamics. Expert knowledge of computing free energy and phase equilibria using molecular simulations. Seeking a position in a research team that works on problems related to my skills and interests.

EDUCATION

PhD	Indian Institute of Science, Bangalore Department: Chemical Engineering CGPA: 6.5/8.0	October 2020 (Thesis Submitted)
ME	Indian Institute of Science, Bangalore Department: Chemical Engineering CGPA: 6.2/8.0	June 2011
BTech	University College of Technology Osmania University, Hyderabad Department: Chemical Engineering Percentage: 75.10	April 2009

SKILLS

Technical:
Molecular dynamics simulations, Monte Carlo simulations, Free energy computation, Phase equilibria computation, Solubility computation, vapor-liquid/ solid-liquid/ vapor-solid interface properties, High performance computing
Programming: Fortran, Python, Shell scripting, LaTeX
Softwares/Packages: LAMMPS, GROMACS, MATLAB, VMD

RESEARCH EXPERIENCE

PhD Research **Aug 2014 – Present**

- Developed a robust statistical thermodynamic based theory to model the gas hydrate phase equilibria with the help of molecular simulations.
- Developed a method to compute solubility of TBAB semi-clathrate hydrates using molecular simulations to evaluate a suitable force field so that semi-clathrates can be studied for potential applications in energy storage and separation processes.

- Presently studying the problem of blockage of natural gas pipelines due to formation of gas hydrates using anti-agglomerants with the help of molecular simulations.
- Presently studying ligand coated gold nanoparticles using molecular simulations to understand the effect of many-body interactions.
- Presently studying crystal nucleation from its solution to understand the molecular mechanism involved with the help of molecular simulations.

ME Research **Aug 2009 – June 2011**

- Studied the drawbacks of existing thermodynamic theories of gas hydrates using molecular simulations.

PUBLICATIONS

1. **Shivanand K. Veesam** and Sudeep N. P.: Computation of the dissociation temperature of TBAB semi-clathrate in an aqueous solution using molecular simulations, *J. Phys. Chem. B* (2020), 124, 9195-9203.

2. Ravi K R A, **Shivanand K. Veesam**, and Sudeep N. P.: Review of the Frenkel-Ladd technique for computing free energies of crystalline solids, *Molecular Simulation* (2020), DOI: 10.1080/08927022.2020.1775221, Just accepted article.

3. **Shivanand K. Veesam** and Sudeep N. P.: vdWP-FL: An Improved Thermodynamic Theory for Gas Hydrates with Free-Energy Contributions due to Hydrate Lattice Flexibility, *J. Phys. Chem. C* (2019), 123, 26406-26414.

4. **Shivanand K. Veesam**, Srikanth R, and Sudeep N. P.: Recent advances in thermodynamics and nucleation of gas hydrates using molecular modeling, *Current Opinion in Chemical Engineering* (2019), 23, 14-20.

5. Hrushikesh Pimpalgaonkar, **Shivanand K. Veesam**, and Sudeep N.P.: Theory of gas hydrates: Effect of the Approximation of Rigid water lattice, *J. Phys. Chem. B* (2011), 115, 10018-10026.

6. **Shivanand K. Veesam** and Sudeep N. P.: Molecular simulation study on inhibition of gas hydrates using anti-agglomerants (Under preparation)

7. Dinesh C, **Shivanand K. Veesam**, Emanuele B, Lara F, Sudeep N. P.: Modeling of effective interactions between ligand coated gold nanoparticles (Ready to submit)

CONFERENCE PRESENTATIONS

1. **Shivanand K. Veesam** and Sudeep N. P.: Improving the robustness of the van der Waals and Platteeuw theory for gas hydrates, ***10th Liblice conference on statistical mechanics of liquids***, SRNI, Czech Republic on June 17-22, 2018.

2. **Shivanand K. Veesam**, and Sudeep N.P: Theory of Gas Hydrates: Effect of the Approximation of Rigid Water Lattice, ***AIChE Annual Meeting***, Pittsburgh, PA, 2012.

3. **Shivanand K. Veesam** and Sudeep N. P.: On the Approximation of Rigid Water Lattice in van der Waals and Platteeuw Theory, ***7th International Conference on Gas Hydrates***, Edinburgh, Scotland, United Kingdom, 2011.

4. **Shivanand K. Veesam** and Sudeep N. P.: Phase Equilibria for Clathrate Hydrates using Monte Carlo Simulation, ***International symposium on Recent and Emergent Advances in Chemical Engineering*** (REACH), IIT Madras, Chennai, India, 2010.

ACCOMPLISHMENTS

Best Poster Award 2019
Inhouse Symposium, Chemical Eng., IISc

Kumar – Gandhi Award 2011
Inhouse Symposium, Chemical Eng., IISc

All India Rank – 173 2009
GATE – 2009, Chemical Engineering

OTHER PROFESSIONAL EXPERIENCE

Teaching Assistant, IISc **Jan 2018 – April 2018**
- Assisted students for the Statistical Thermodynamics course

Teaching Assistant, IISc **Aug 2017 – Dec 2017**
- Assisted students for the Thermodynamics course

Adhoc Faculty, NIT, Warangal **Jan 2013 – May 2014**
- Faculty instructor for Thermodynamics, Chemical Reaction Engineering, and Fluid Mechanics courses

Project Assistant, IISc, Bangalore **July 2011 – June 2012**
- Worked on implementing Molecular dynamics techniques in the package developed in our group.

REFERENCE

Prof. Sudeep N Punnathanam
Chemical Engineering,
Indian Institute of Science, Bangalore – 560012
Phone: +91- 80-2293 3109, Email: sudeep@iisc.ac.in