Prathamesh D. Raiter

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Education

- **Cornell University** — Ithaca, NY
  M.S. in Materials Science and Engineering — **GPA: 3.99/4.00**
  Minor: Computational Science and Engineering — *August 2018 – July 2020 (Expected)*

- **Institute of Chemical Technology** — Mumbai, MH, India
  B. Tech. in Polymer Engineering — **GPA: 8.28/10.0**
  Minor: Chemical Engineering — *August 2014 – May 2018*

Research Experience

- **Molecular dynamics investigation of electric field modulated polymers** — Master's Thesis
  Advisor: Prof. Meredith Silberstein — *September 2018 - Present*
  - **Modeling**: Built 12 initial configurations of ionically charged polymers (with variable repeating units, chains, ions) as gaussian chains with excluded volume effect, using Python, for coarse-grained and all-atom simulations.
  - **Simulation**: Simulated uniaxial tensile deformation of coarse-grained and all-atom models under electric field.
  - **poly_ana**: Developed a python library to post-process and analyze uniaxial tensile deformation simulation data.
  - **Self-regulation of mechanical properties**: Analyzing influence of polymer rigidity, charge density, free ions, solvent and concentration of ionic bonds on molecular assembly and mechanical properties under electric fields
  - **Multiphysics modeling of polymers**: Validation of MD findings using Reverse Addition-Fragmentation polymer synthesis, solution-based experiments, spectroscopy and mechanical testing.

- **Stine Research Center, FMC, Newark, DE** — *Computational Science intern*
  Advisor: Dr. Laurie Christianson — *June 2019 - August 2019*
  - **Machine learning**: Constructed bayesian, support vector machines and random forest models for active/inactive compounds in Level 2 and Level 3 biological screens for insecticides, herbicides, nematicides and fungicides.
  - Purchased new compounds worth 23,600$ for Level 1 high-throughput screens based on the Bayesian model.
  - **Theoretical spectra**: Developed an integrated workflow in python and shell, with pipeline pilot as frontend, to compute theoretical pKa, UV/Vis and NMR spectra using Time-dependent DFT for *any* chemical compound.
  - Theoretical spectra computation allowed chemists to conveniently run UV/Vis on hypothetical compounds earlier in a project, enabling them to avoid synthesis of compounds not showing photostability outdoors.

- **Design, Synthesis and Evaluation of Rivastigmine Transdermal Patches** — Senior Thesis
  Advisor: Prof. Shashank T. Mhaske, Prof. Pradeep R. Vavia — *September 2017 - May 2018*
  - **Patent hunt**: Chose a set of rivastigmine compatible monomers based on a commercial product's patent search.
  - **Terpolymerization**: Synthesized a 2-EHA, acrylic acid and methyl acrylate terpolymer with free radical solution polymerization to achieve accurate adhesive and cohesive strength for a 24-hour drug in adhesive patch.
  - Determined the reactivity ratios, reaction temperature and time based on a 2^2 *full factorial experimental design.*
  - **Characterization**: Characterized the terpolymers with DSC, FT-IR and XRD. Compared peel Strength, adhesive transfer and assay for drug in adhesive patches made with commercial product and synthesized terpolymer.
  - **Properties**: Synthesized drug in adhesive patch had adhesion and stability similar to the commercial product.

- **BASF Innovation Center, Turbhe, Mumbai** — *Coatings Research intern*
  Advisor: Dr. Parag Gaikwad — *May 2017 - July 2017*
  - **Testing**: Compared Dirt Pick-Up Resistance, elongation, elasticity, tensile strength, toughness, hardness and fracture toughness for a BASF Styrene based architectural coating dispersion and a competitor's product.
  - **Flexibility**: Increased crack-bridging ability and elongation for BASF coating by modifying rheological additives.
  - Characterization using UTM, Rheometer, Accelerated Weathering Tester, Spectrophotometer, Rectified bubbling.

- **Synthesis and characterization of Zinc Oxide nanoparticles** — Undergraduate Research Project
  Advisor: Prof. Ramanand N. Jagtap — *May 2017 - July 2017*
  - **Precipitation**: Synthesized nano ZnO and correlated its size with the reaction conditions and precipitation synthesis routes present in literature. Particle size analyzer confirmed nanostructures for prepared ZnO.
  - Characterizated the precipitated nano ZnO with Particle size analyzer, XRD and UV-Vis spectroscopy.
  - XRD patterns showed that ZnO nanoparticles have hexagonal unit cell structure.

Honors and Awards

- DST-India INSPIRE Scholarship for Higher Education for being in the top 1% of class 12 board exam (2014).
- P-Pack 2017 winner, a National level *Polymers in Packaging* quiz organized by Indian Plastics Institute.
- Branch *Rank 1* for Semester V (Fall 2016) and Semester VI (Spring 2017) among 17 students.
- Awarded *Best Intern* at BASF Innovation Center, Mumbai out of 9 interns.
- *High Distinction* in Australian National Chemistry Quiz (2008, 2009, 2010, 2011, 2013)

Skills

- **Simulation**: Molecular Dynamics, Monte Carlo methods, Density Functional Theory, Quantum Mechanics
- **Software**: Pipeline Pilot, KNIME, Biovia Materials Studio, Schrodinger Jaguar and MacroModel, GROMACS, LAMMPS, RDKit, PyMOL, VMD, Adobe Photoshop, Premiere Pro, InDesign
- **Languages**: *Proficient* - Python, MATLAB, Shell scripting, HTML *Familiar* - C/C++, Java, Perl
- **Analytical**: FT-IR, NMR, MS, DSC, UV-Vis Spectroscopy, HPLC, XRD, GPC, TGA

Select Coursework

- **School**: Statistical Mechanics, Principles of Molecular Simulation, Computational Materials Science, Design of Experiments, Machine Learning, Spectroscopic techniques, Shell scripting, Learning with big data
- **Online**: Polymer Physics, Object-oriented Programming, MPI Foundations, GPU Programming, HPC

Professional Memberships

American Physical Society (APS), New York Academy of Sciences (NYAS), American Chemical Society (ACS)

Poster Presentations

- *Bayesian Classification of Level2/Level3 Actives and Theoretical Computation of UV/Vis Spectra* at Stine Research Center, FMC (Global Research and Development), Newark, DE.
- *Coatings in Marine Industry* at Advances in Polymers and Coatings, Rangotsav 2017, ICT, Mumbai.
- *Cost-effective solution to metallize Polyethylene* at Industry Defined Problem, Vortex 2016, ICT, Mumbai.

Certifications and Activities

- Open-source contributor to *MDAnalysis* and *MDTraj* Github.
- Certified grade A at 15-week *UAA-ICT Certificate Course in Practice of Chemical Technology* conducted by UDCT Alumni Association (UAA), ICT, Mumbai in January-April 2017.
- Designed and constructed a working model of 1,1 - Shell and Tube Heat Exchanger (78% experimental efficiency) considering a multi-component Sieder Tate laminar flow for Chemergence 2016, TSCE, Mumbai.
- Designed and constructed a working model of an elementary eco-friendly rocket stove for use in rural India and demonstrated it at Vortex 2016, ICT, Mumbai
- ICT Debate Club, Badminton Club and Hiking Club.

Leadership and Service

- **Cornell Center for Materials Research Outreach**: Science activity demonstrator at *Family Science Event*, first Saturday of each month, at Tompkins County Public Library, Ithaca, NY since September 2018.
- **Mechanics for Material Design lab**: Polymer cross-links booth instructor in 4-H Youth building at NY State Fair, August 2019.
- **Hindustan Times Clean My Mumbai**: Cleaned a two-kilometer eastern stretch of the Powai lakefront along with Bandra Cycle Club, as a part of HT Clean My Mumbai initiative.
- **In-Plant Training Coordinator, ICT 2016-2017**: Engaged students with the industries they were interested to intern at, and encouraged companies to take up captivating summer projects with students.