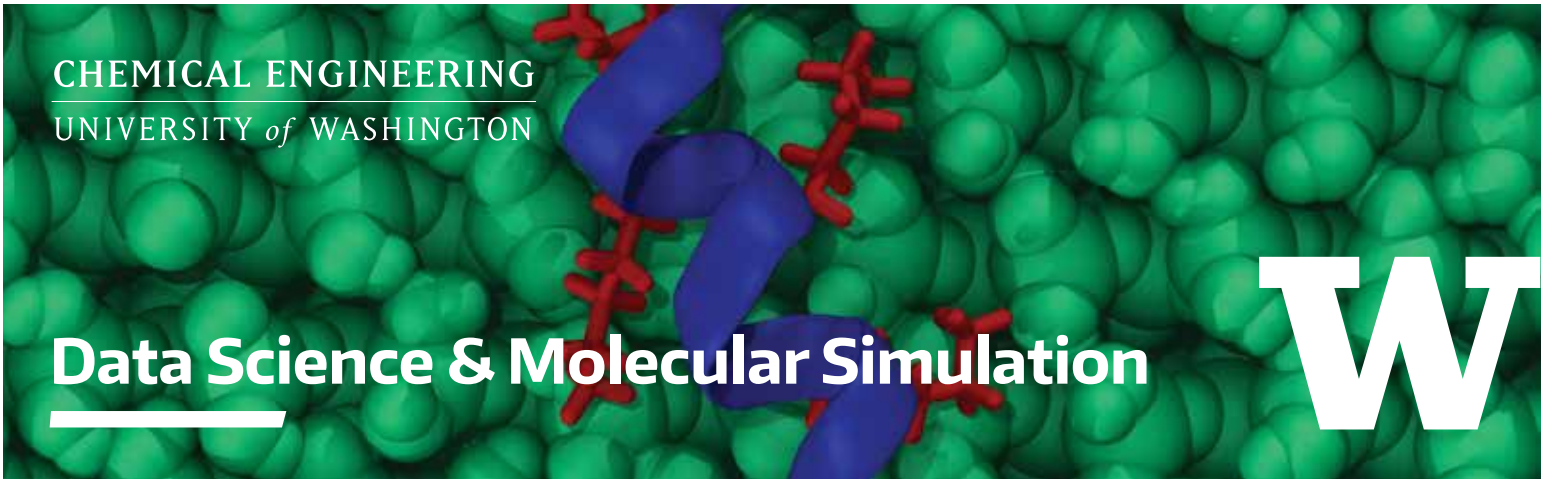

CHEMICAL ENGINEERING
UNIVERSITY of WASHINGTON

# Data Science & Molecular Simulation

**Ever-expanding streams of data** from high-throughput experiments, industrial sensors, advanced instrumentation, and simulation are fundamentally changing chemical engineering. Our faculty are at the forefront of this data science transformation. They're using machine learning, computational molecular science, and high-performance computing to improve semiconductors and solar cells, characterize materials, and discover novel renewable chemicals, among other cutting-edge projects.

Above: Helical peptide LK(alpha)14 adsorbed on the surface of quartz through lysine interactions, created by Janani Sampath

## Featured research clusters

### Molecular simulation

We utilize molecular- and quantum-mechanics simulations to understand how molecules behave and interact in complex settings. We also build new methods and tools for enhanced sampling and scalable data analysis. Our simulations serve a variety of application spaces including human health, energy and the environment.

### High-throughput experimentation and data analytics

Our research enables combinatorial sampling, screening and adaptive online high-throughput experimentation for identifying promising molecules and materials for cutting edge applications: photonic and electronic energy conversion and storage, medicine, and more.

### Molecular design

We create and employ cutting edge molecular data science methods such as machine learning for the design of new molecules and materials. Example applications include pharmaceuticals, energy storage, and separations.

### Reaction engineering

The atomistic motion of reactant molecules governs chemical reactivity. We create and apply methods which combine ab initio simulations with machine learning to accelerate the design of kinetics. Our research has a broad range of applications, from drug and catalyst design to industrial reactors.

**Neda Bagheri**

**David Beck**

**James Carothers**

**Hugh Hillhouse**

**Jorge Marchand**

**Shachi Mittal**

**Elizabeth Nance**

**Jonathan Posner**

**Lilo Pozzo**

**Daniel Schwartz**

**Zachary Sherman**

## Campus opportunities

eScience Institute
Empowering students and researchers in all fields to answer fundamental questions through the use of large, complex, and noisy data

Research computing infrastructure, including NextGen Supercomputer Hyak

ChemE Advanced Data Science degree option

More at: **www.cheme.uw.edu/research/areas**