Rensselaer

The HOWARD P. ISERMANN
DEPARTMENT OF CHEMICAL AND
BIOLOGICAL ENGINEERING

# CBE Seminar Series – Spring 2025

## Dr. Rajesh Khare

Professor and Whitacre Department Chair
Department of Chemical Engineering
Texas Tech University

## Seminar: Wednesday, April 2, 2025
## 9:30 a.m. (Ricketts 211)

### "From Molecules to Rheology: A Journey across Length and Time Scales"

**Abstract:** Rheology as an engineering science was developed based on experiments and continuum theory. Rheology of complex fluids is governed by their structure, which in turn, depends on the intermolecular interactions in these systems. Molecular simulations offer the unique ability to investigate the relationship between rheology and the molecular structure and interactions in complex fluids. The application of simulations for solving engineering problems in rheology will be illustrated in this presentation.

The first part of the presentation will focus on an approach for overcoming the large time scale gap between molecular simulations and experiments. It is shown that the time-temperature superposition principle from experimental rheology can also be applied to extend the frequency or time scale range of molecular simulation results. The application of this approach to a wide variety of soft matter systems including cross-linked epoxy, asphalt, ionic liquid, and colloids will be discussed. The second part of the presentation will discuss the development of the probe rheology simulation technique which is the simulation analogue of the experimental bead microrheology. The proposed formalism enables determination of the viscoelasticity of soft matter systems by analysis of probe motion. The application of particle rheology for deciphering the connection between system structure and viscoelasticity in a number of systems such as polymer melts, nanocolloidal suspensions, and biofilms, will be discussed.

**Biography:** Rajesh Khare has more than 30 years of experience working in the field of molecular simulations spanning both academia and industry. Following his Ph.D. and post-doctoral research, he worked in various scientific and managerial capacities in the R&D group at Accelrys, Inc. He joined the faculty of Texas Tech University in 2005 where he previously served as the Associate Dean of Research and Graduate Programs in the College of Engineering and is currently the Chair of the Department of Chemical Engineering. The underlying theme of Prof. Khare's research is the innovative use of molecular simulations for studying nanoscale transport phenomena, structure-property relationships in soft matter systems, and thermodynamics of mixtures. An important thrust of Prof. Khare's work is to make quantitative connections between the results of molecular simulations and laboratory experiments.

**Refreshments will be available at 9:00 a.m. in the Ricketts Coonley Lounge.**