

Development of Predictive Models by Chemical Informatics Methods in Polymeric Materials Research (*Faculty Mentor: Bakhtiyor Rasulev*)

The research in Rasulev group is focused on development of predictive models to investigate and design novel bio-based polymeric materials and to predict various properties, including solubility, degradation rate, toxicity, etc. The group applies computational chemistry and cheminformatics methods for modeling, data analysis and development of predictive structure-property relationship models. REU students will learn how to extract chemical data from available public sources, build datasets with structures, and then apply machine learning and cheminformatics tools to investigate and design new chemicals and polymers with improved properties.

