

4) Modeling and Design of the Thermophysical Properties of Novel polyamines and Nanoparticle-Organic Hybrid materials for CO₂ capture

Proposed by Fernando Escobedo

This project entails the use of advanced molecular dynamics simulation methods to predict and correlate the thermophysical properties of novel oligomeric amines adsorbed or tethered on solid substrates, including inorganic nanoparticles. Such materials are the object of intense experimental studies by several groups at Cornell and elsewhere for potential applications involving, for example, the capture of CO₂ and organic gases. This project is part of a joint effort to provide a more fundamental basis to the rational design of these new classes of materials.