Molecular simulations of adsorption of gases in polymeric materials

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In this talk, we will show how to model adsorption behaviour of different fluids (nitrogen, hydrogen, ethane, ethene) on two semicrystalline phases (δ and ε) of syndiotactic polystyrene. These two polymorphs present nanoporosity, being able to adsorb molecules of low molecular weight in their cavities (δ) and channels (ε). By means of Grand Canonical Monte Carlo molecular simulations, adsorption isotherms were calculated, exploring the possibility utilization of these materials with different porpoises; storage, characterization of superficial properties of the adsorbent materials, and separation of a binary mixture of gases.