Poster SCF1

A Statistical Mechanical Equation of State for Critical Property Predictions in Pore-Confined Fluids

Eldred CHIMOWITZ[a], Pedro LOPEZ-ARANGUREN[b], Concha DOMINGO[b]
[a] *University of Rochester, Rochester, NY, UNITED STATES,* [b] *Instituto de Ciencias de Materiales de Barcelona, Barcelona, SPAIN*

✉Chim@che.rochester.edu

Our poster will present results discussing the theoretical basis for a novel equation of state intended for use in calculating the thermodynamic properties of both bulk and pore-confined supercritical fluids. The model arises from a rigorous statistical mechanical treatment of the effects of pore-confinement on the thermodynamic behavior of fluids. It is of the mean-field genre and applicable to both bulk and pore-confined fluid systems. We illustrate its use, and advantages, over other widely used equations of state used for bulk property predictions in supercritical fluids. In particular though, our model goes over seamlessly to the situation where a fluid is adsorbed in a porous medium. We provide results for this type of system and illustrate the model's accuracy by comparing its thermodynamic predictions to experimental adsorption data for both carbon dioxide and propane adsorbed in highly porous silica aerogels.

Keywords

Critical phenomena, confined fluids, porous media, adsorption, separations.