Impact of Geometrical Disorder on Phase Equilibria of Fluids and Solids Confined in Mesoporous Materials

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Mesoporous solids used in practical applications or naturally occurring porous materials often possess structural disorder over broad length scales. Understanding structural disorder is important in many context because it determines many properties of the substances confined in their pore spaces. Gas sorption and thermoporometry methods remain most powerful and widespread approaches for assessing structural properties of such materials. The basic assumption typically made within the conventional models used for the analysis is the representation of complex pore networks as collections of independent pores. In my talk I will first discuss the validity of this assumption and show how a simple physical connection between two pores with different pore sizes gives rise to novel phenomena in phase transitions, such as in capillary-condensation or freezing, which are absent in the conventional models. Thereafter, I introduce a simplistic model mimicking the most essential properties of disordered pore networks, namely a serially-connected pore model represented by a linear chain of statistically joined single pores, for which the phase equilibria can be predicted analytically. By correlating its predictions with various experimental observations, I will show that this model gives notable insight into collective phenomena in phase-transition processes in disordered materials and is capable of explaining self-consistently the majority of the experimental results obtained for gas−liquid and solid−liquid equilibria in mesoporous solids. The implications of the model, including its pitfalls, for improving the accuracy of the structural analysis of mesoporous materials will also be discussed.

1. D. Schneider, R. Valiullin, Capillary Condensation and Evaporation in Irregular Channels: Sorption Isotherm for Serially Connected Pore Model, The Journal of Physical Chemistry C, 123 (2019) 16239-16249.
2. H.R.N.B. Enninful, D. Schneider, D. Enke, R. Valiullin, Impact of Geometrical Disorder on Phase Equilibria of Fluids and Solids Confined in Mesoporous Materials, Langmuir, 37 (2021) 3521-3537.