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## Colloquium

### **Condensation of methane in metal organic frameworks (MOFs): Novel phase transitions in an ordered porous medium**

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Metal-Organic Frameworks (MOFs) are nanoporous crystalline materials where metal oxide complexes are connected to each other by organic linkers. Due to the large inner surface, MOFs are well-suited for applications associated with gas adsorption. Experimentally, adsorption isotherms have been extensively studied for molecules such as methane, carbon dioxide, water, etc., indicating the possibility of a phase transition in various MOF structures. However, the nature of these transitions is not well understood, in particular with respect to the interplay between layering on the inner MOF surface and gas-liquid coexistence in the porous structure.

We use grandcanonical Carlo simulations in combination with successive umbrella sampling to study the condensation of methane in various MOF systems with different porosities. In each system, two phase transitions and thus two critical points are found. We characterize the coexisting phases and show that these transitions belong to the 3D Ising universality class.

***Friday, Feb 27<sup>th</sup> 2015***

***4:00 PM (Tea/Coffee at 3:30 PM)***

***Seminar Hall, TCIS***