

Fluids in mesopores. A new theory and its applications

Harald Morgner

Wilhelm-Ostwald Institute for Physical and Theoretical Chemistry, University Leipzig, 04103
Leipzig, Germany. *E-mail*: hmorgner@rz.uni-leipzig.de

Over the last few years, we have worked out a new theory for “Thermodynamics of Confined Systems”. A first version of this theory has been shown to explain the key experiments in this field [1]. A short outline of the fully developed new theory will be presented at the workshop as basis for discussing a few applications. Further, it will be shown, that the theory allows simulating diffusional and convectional transport (nanofluidics) at the same time without the need to introduce capillary forces (surface or interface tensions) by phenomenological parameters.

The second part of the talk is devoted to the potential for practical use. It turns out that the new theory does not only remove conceptual problems, but at the same time opens the route to a number of new states found in porous systems which may lead to improved applications. In particular we will focus on the possibility to drive a fluid in a pore into exotic states under static and under dynamic conditions. E.g. it turns out that states with negative pressure can be reproducibly controlled, provided one has full control over the phenomenon of adsorption hysteresis. Negative pressure states are in principal known since the time of Torricelli and they have been discussed in the literature [2, 3] as experimentally accessible situations. Still, they have not been turned into practical usefulness which is likely to be caused by the notion of their metastability in macroscopic systems.

Possible applications refer to controlling chemical reactions as well as new routes to energy efficient separation processes.

References

1. H. Morgner *Computer simulation on static and dynamic properties during transient sorption of fluids in mesoporous materials*, J.Phys.Chem.C 114 (2010) 8877-83
2. A. R. Imre *On the existence of negative pressure states*, Phys. Stat. Sol. (b) **244** (2007) 893-9
3. A. R. Imre et al. *Indirect methods to study liquid-liquid miscibility in binary liquids under negative pressure* NATO Science Series II, Mathematics, Physics and Chemistry (2007) 242 (Soft Matter under Exogenic Impacts) 389-98