

# 多相学术论坛（第二期）

## CALCULATING THE PRESSURE TENSOR IN THIN ADSORBED FILMS

时 间： 2016年9月26日（星期一） 16:00-17:30

地 点： 过程大厦308会议室

主持人： 张锁江

报告人： Prof. Keith E. Gubbins



W.H. Clark Distinguished University Professor,  
Member of National Academy of Engineering

*Department of Chemical & Biomolecular Engineering,  
North Carolina State University,  
Box 7905, Raleigh, NC 27695-7905, U.S.A.*

### 报告简介：

There is an abundance of anecdotal evidence that nanophases adsorbed within nanoporous materials can exhibit high pressures as a result of the confinement<sup>1,2</sup>. For example, phase changes and chemical reactions that only occur at high pressures in the bulk phase occur in the confined phase at bulk phase pressures that are orders of magnitude lower. The pressure in the pore is a second order tensor, and for simple pore geometries has both a normal pressure component (normal to the walls) and one or more tangential components (parallel to the walls).

For simple fluids in pores that are up to a few nanometers in width, molecular simulations show that both the normal and tangential pressures can be locally very high (thousands or tens of thousands of bars) in the pore, even though the bulk phase in equilibrium with the pore is at a pressure of one bar or less. The cause of these high in-pore pressures will be discussed, and where possible comparison with experimental results will be made<sup>3</sup>.

When the molecules in the confined nanophase react with each other chemically, or with the pore walls, it may be possible to achieve even higher tangential pressures, in the megabar range. Evidence for this is provided by recent experiments on sulfur (an insulator at ambient conditions) in narrow single-walled carbon nanotubes, carried out by Kaneko and coworkers<sup>4</sup>. They find that the sulfur atoms within the pore covalently bond to form a one-dimensional phase that is metallic. In the bulk phase sulfur forms a metallic phase only at pressures above 95 GPa. In our recent molecular dynamics simulations of this system we find that the sulfur atoms are covalently bonded in the pore and that they experience tangential pressures in excess of 100 GPa as a result of the strong confinement.

<sup>1</sup> Yun Long, Jeremy C. Palmer, Benoit Coasne, Małgorzata Śliwowska-Bartkowiak and Keith E. Gubbins, "Pressure enhancement in carbon nanopores: A major confinement effect", *Physical Chemistry Chemical Physics*, **13**, 17163-17170 (2011).

<sup>2</sup> Yun Long, Jeremy C. Palmer, Benoit Coasne, Małgorzata Śliwowska-Bartkowiak, George Jackson, Erich A. Müller and Keith E. Gubbins, "On the Molecular Origin of High Pressure Effects in Nanoconfinement: Effects of Surface Chemistry and Roughness", *Journal of Chemical Physics*, **139**, 144701 (2013)

<sup>3</sup> H. Drozdowski, M. Kempinski, M. Śliwowska-Bartkowiak, M. Jazdzewska, Y. Long, J.C. Palmer and K.E. Gubbins, "Structural Analysis of the Behavior of Water Adsorbed in Activated Carbon Fibers", *Physical Chemistry Chemical Physics*, DOI: **10.1039/C2CP22111J** (2012).

<sup>4</sup> Y. Fujimori, A. Morelos-Gómez, Z. Zhu, et al., "Conducting Linear Chains of Sulphur Inside Carbon Nanotubes", *Nature Comm.*, **4**, DOI 10.1038/ncomms3162 (2013).