SAND2014-1872C

American Chemical Society 247th Meeting

Nanogeochemistry: Nanostructures, emergent properties, and their implications to chemical reactions and mass transfers

Yifeng Wang

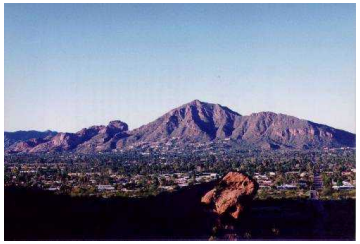
Sandia National Laboratories

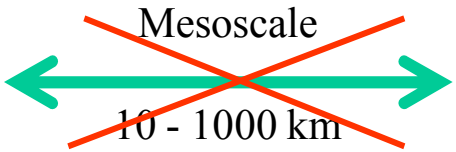
Albuquerque, New Mexico, USA

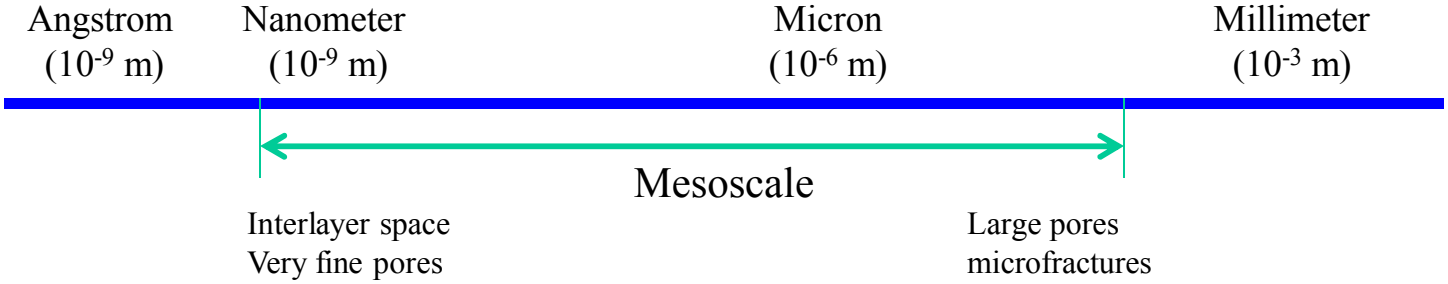
Sandia National Laboratories

Mesoscale

What is the mesoscale?





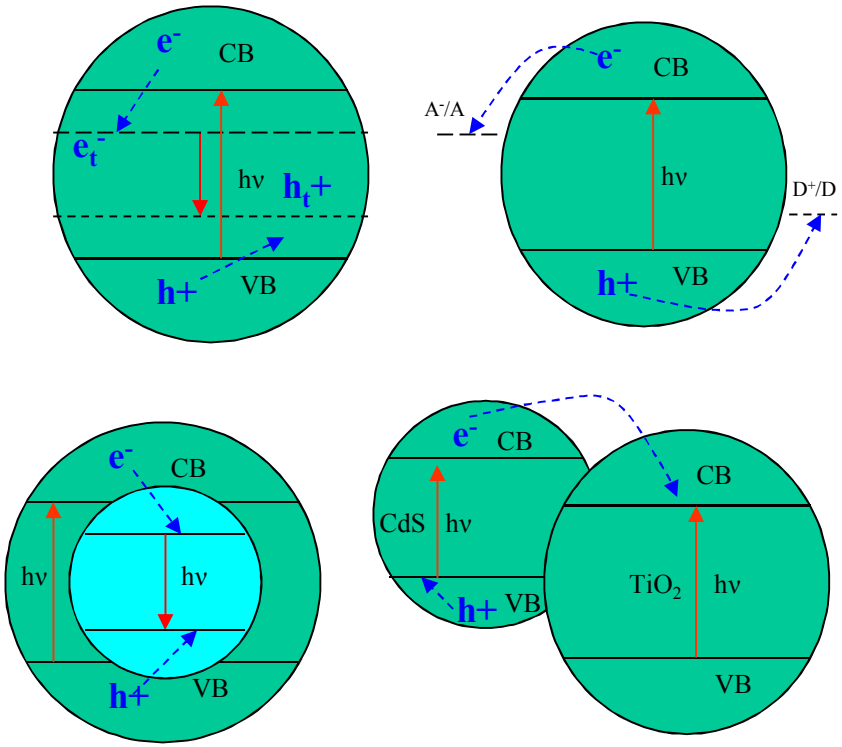


Why mesoscale?

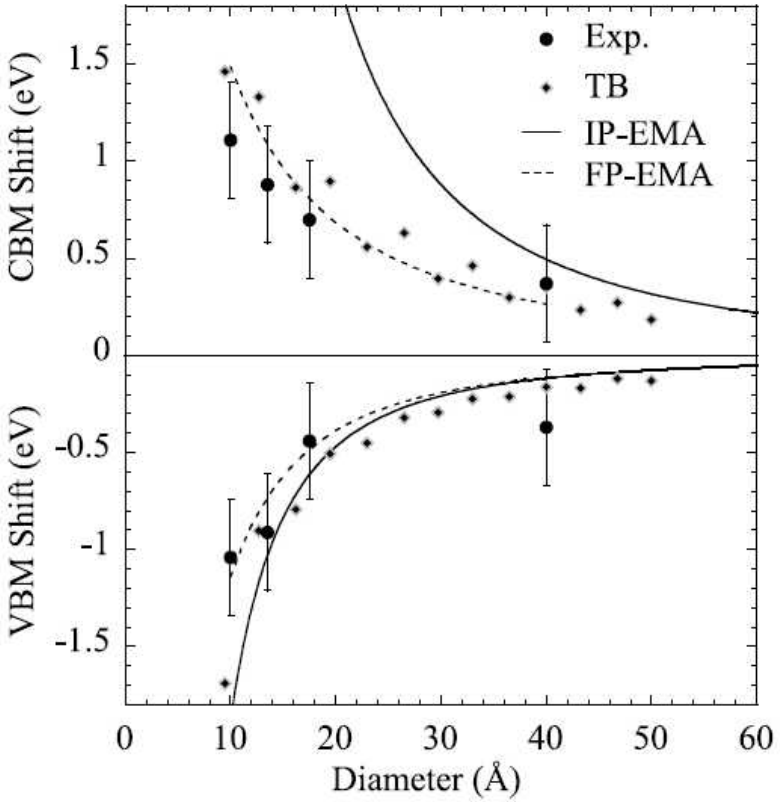
- Emergent properties
- Key linkage between micro to macro (e.g. Wang et al., 2012, ES&T)

Sandia National Laboratories

Size-Dependent Material Properties



Photophysical/Photochemical Processes
in Semiconductor Nanoparticles
(Roduner, 2006)

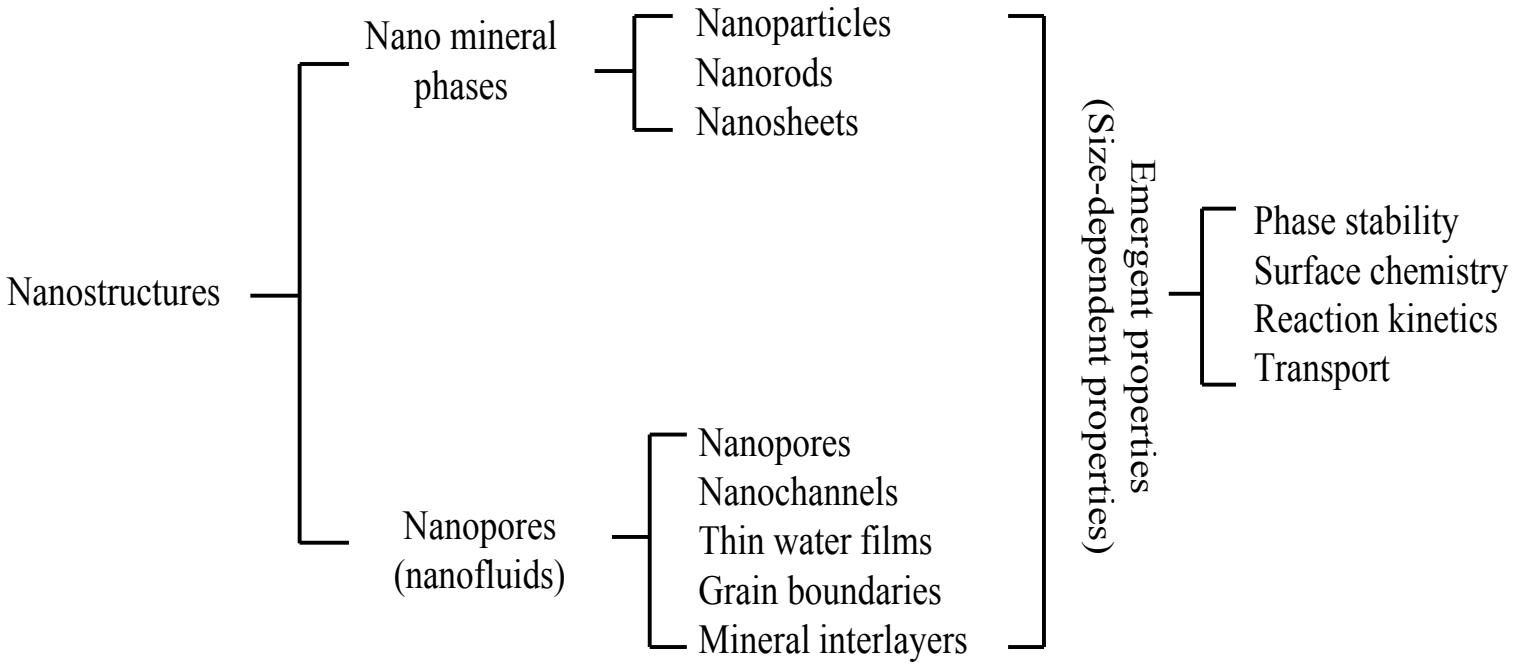


Size-dependent CdS band gap

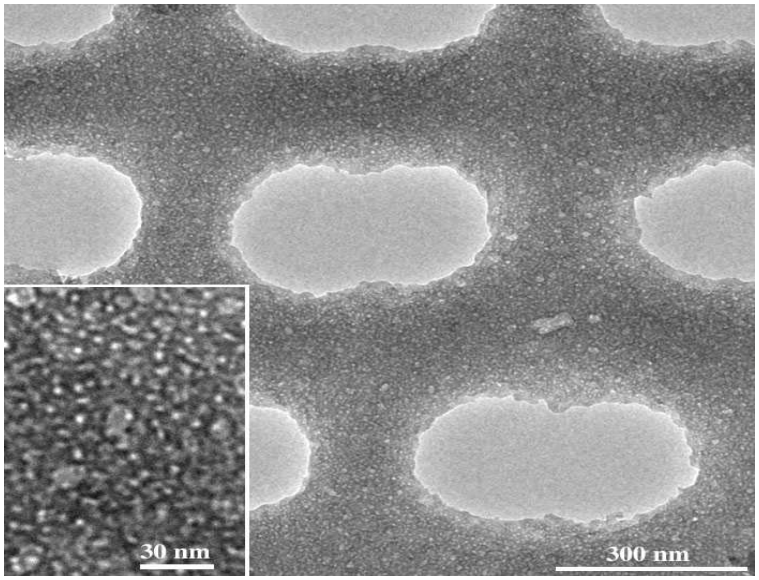
(Lüning et al., 1999, Sold State Communication)

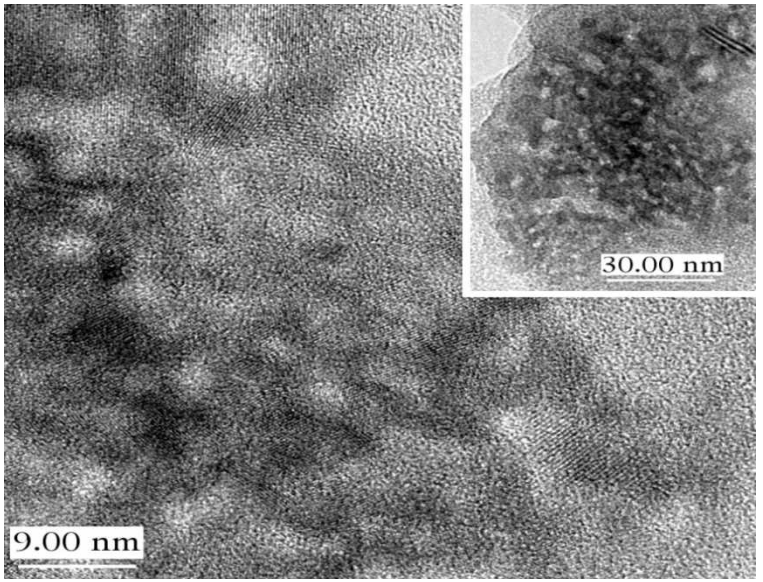
Sandia National Laboratories

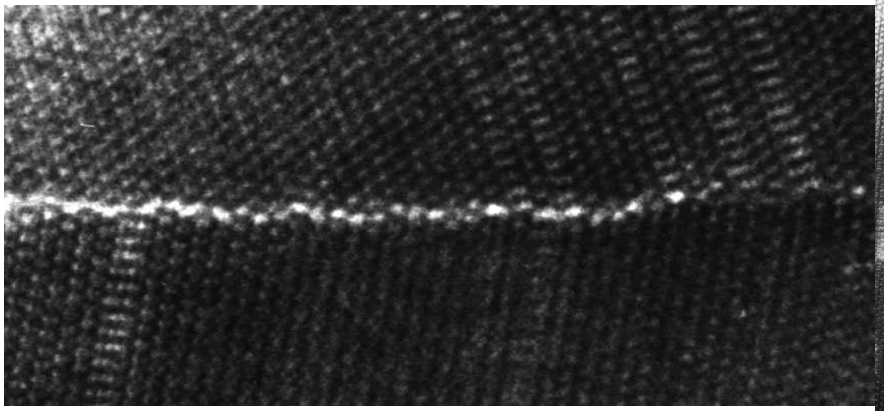
Systematics of Nanogeochemistry

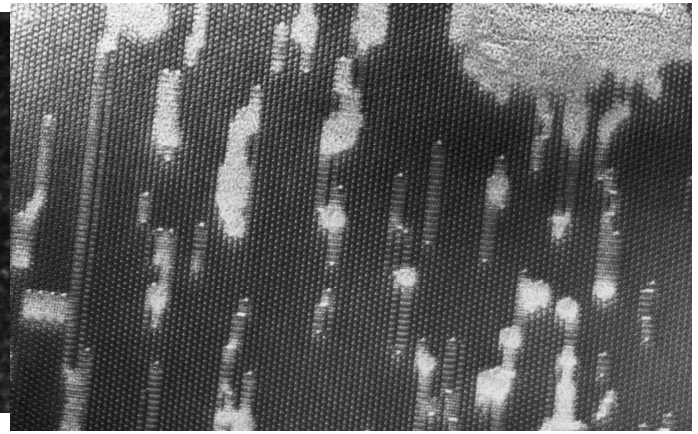


Nanopores in Geologic Materials





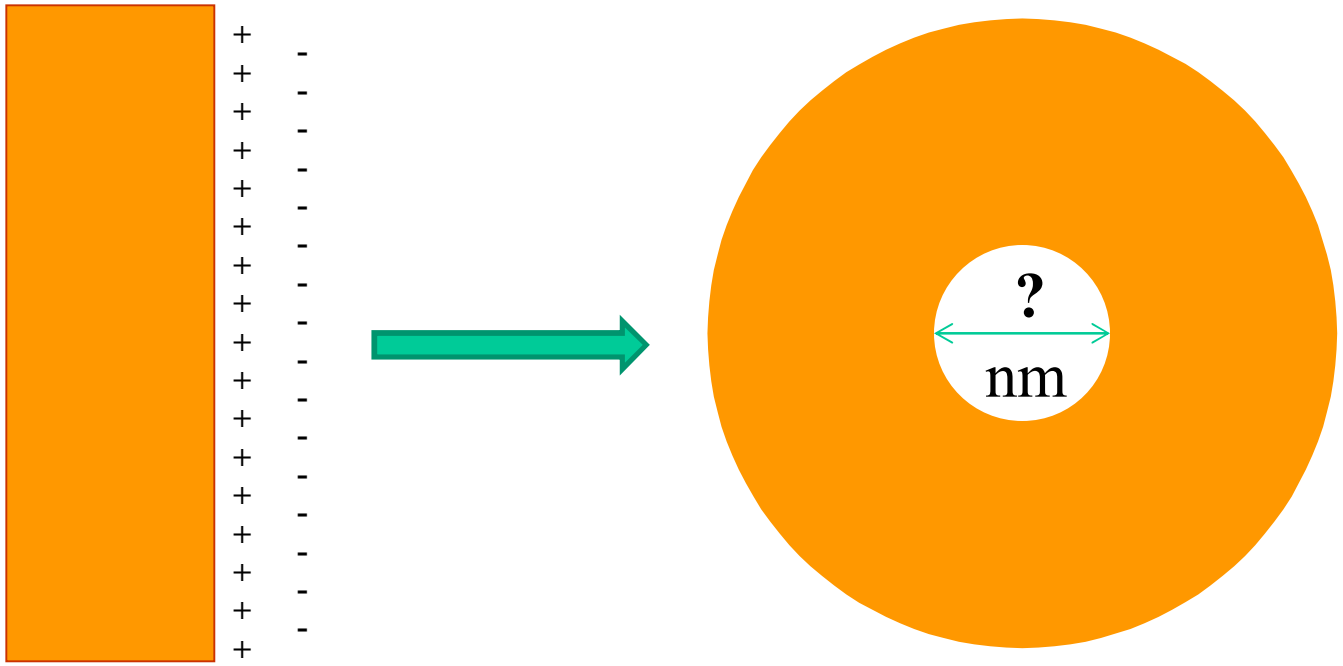




Wang et al., 2003, Geology

Sandia National Laboratories

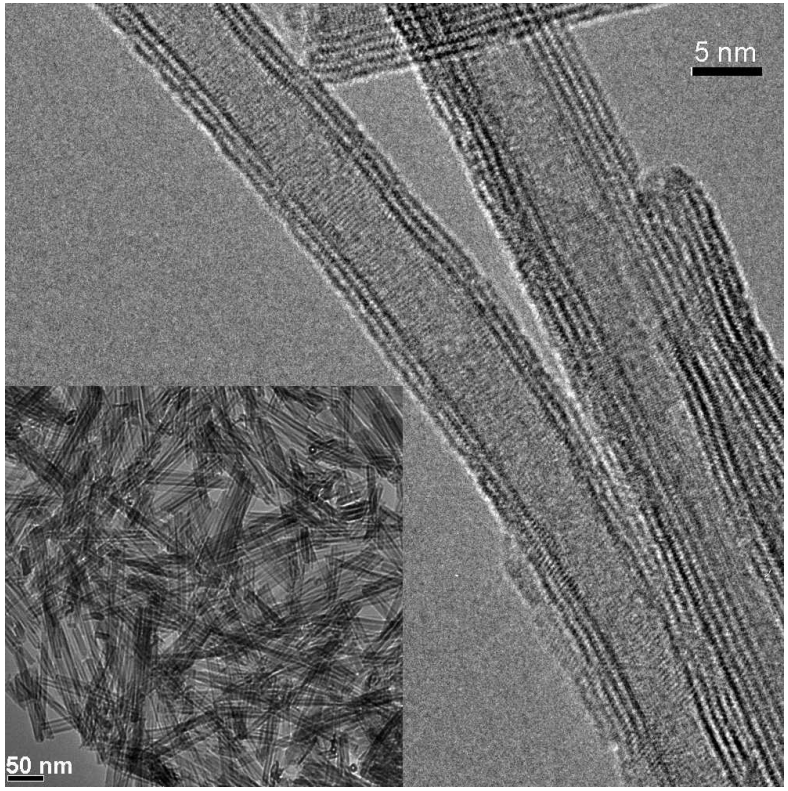
Confined vs. Unconfined Surface

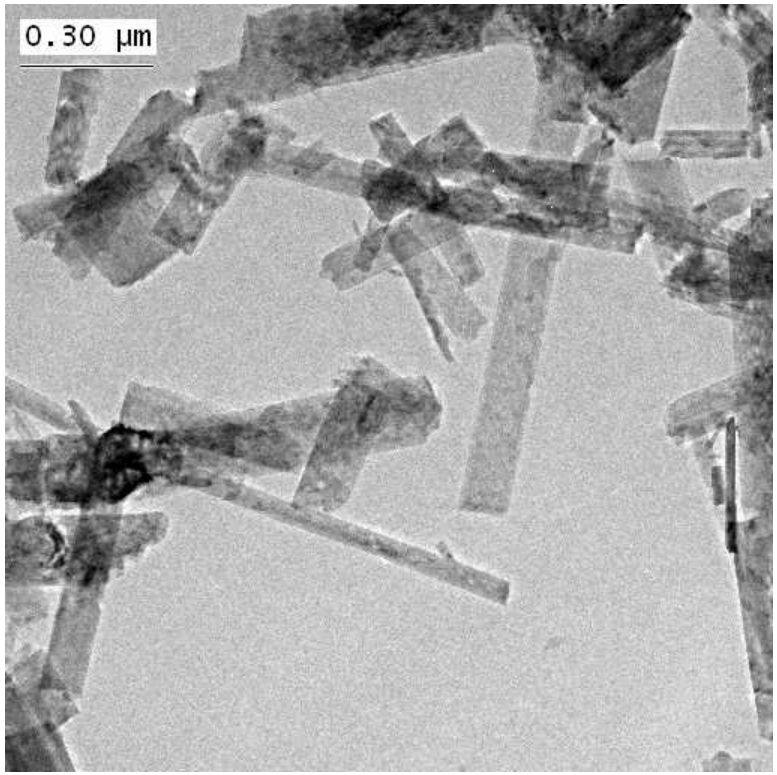


Unconfined

Confined

Synthesis of TiO_2 Nanotubes and nanorods

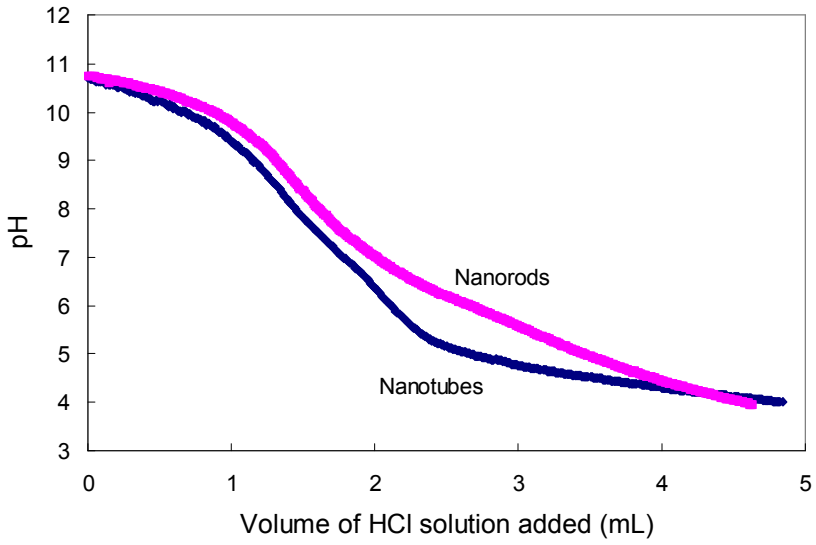


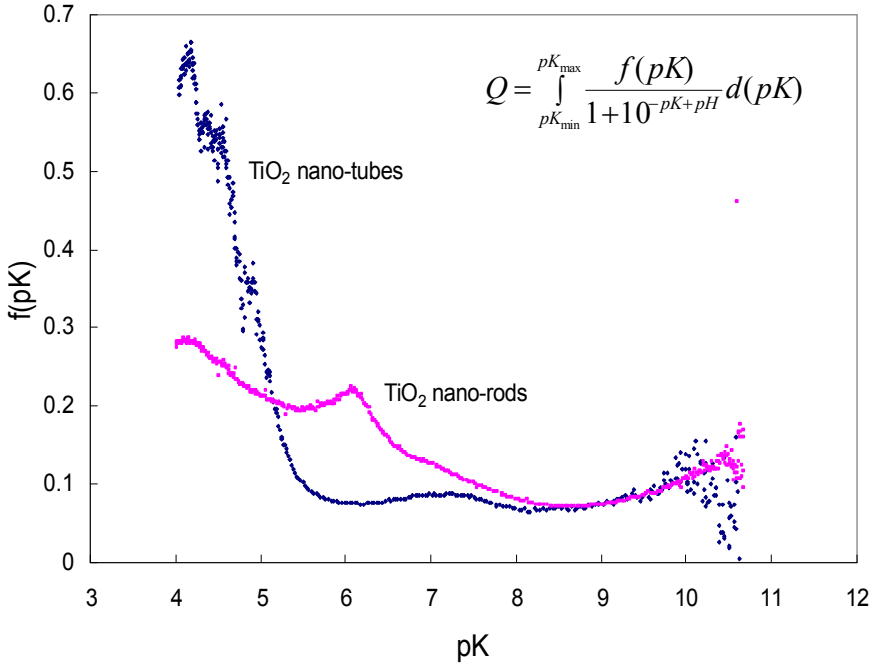


Wang et al. (2008)

Sandia National Laboratories

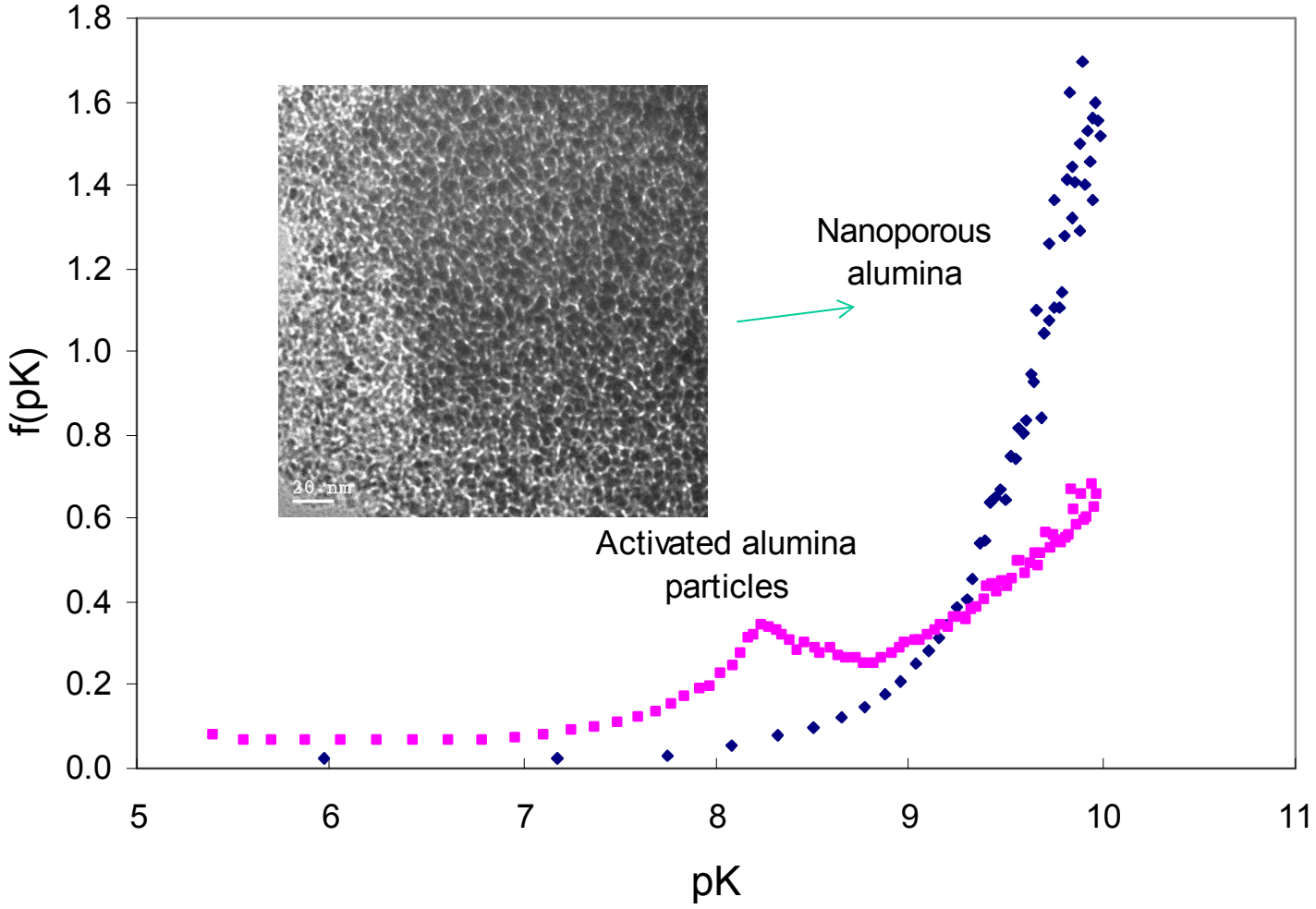
Distribution of Acidity Constant





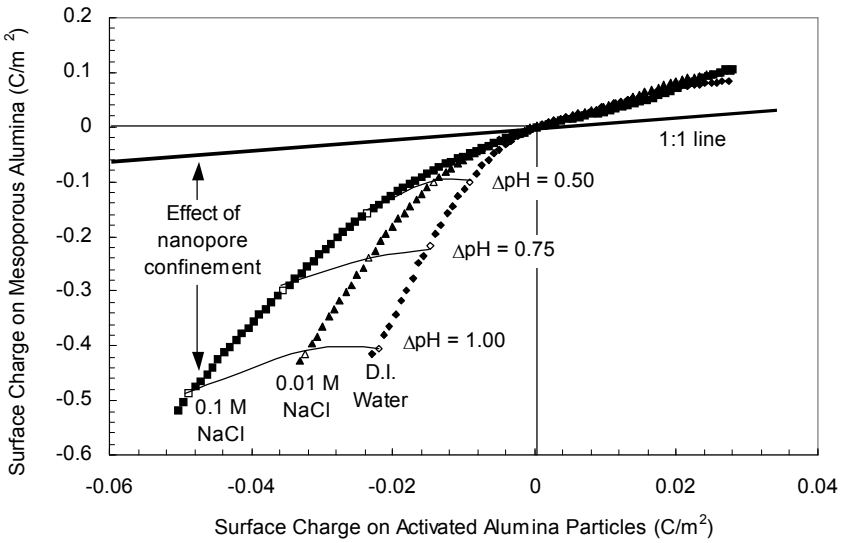
Sandia National Laboratories

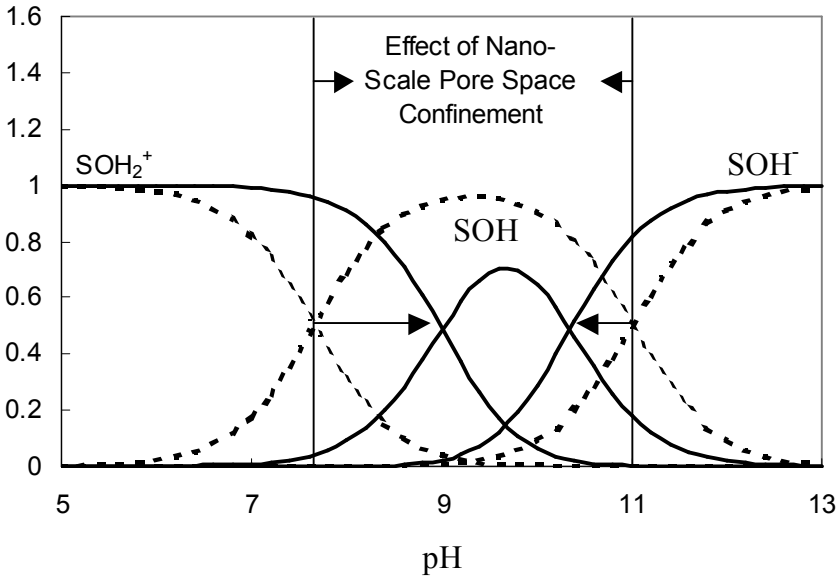
Distribution of Acidity Constant



Sandia National Laboratories

Effect of Nanopore Confinement on Surface Chemistry





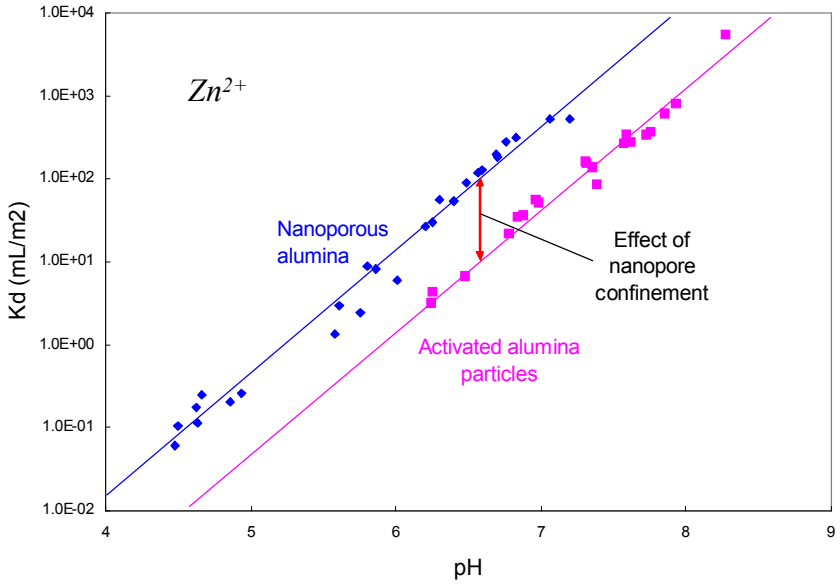
Nanoporous alumina has a higher surface charge density, which is less sensitive to ionic strength changes.

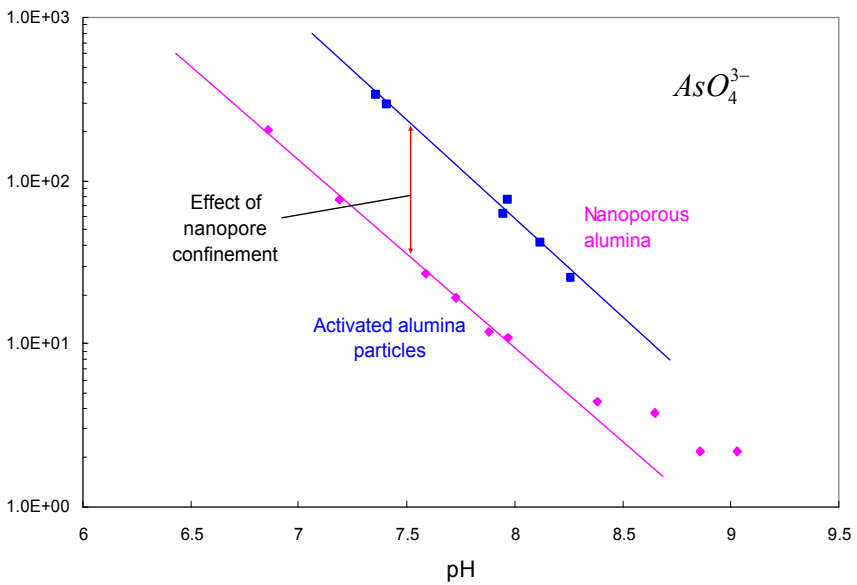
Nanopore confinement causes a solid-water interface to be more either positively or negatively charged.

Wang et al., 2002, JCIS; 2003, Geology

Sandia National Laboratories

Nanopore Confinement and Ion Sorption



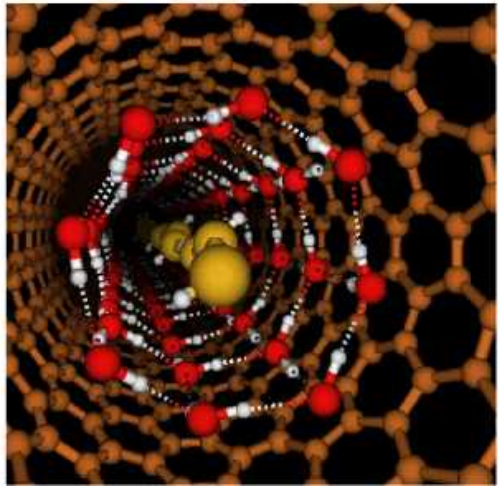


Nanopore confinement enhances ion sorption onto a solid-water interface for both cations and anions.

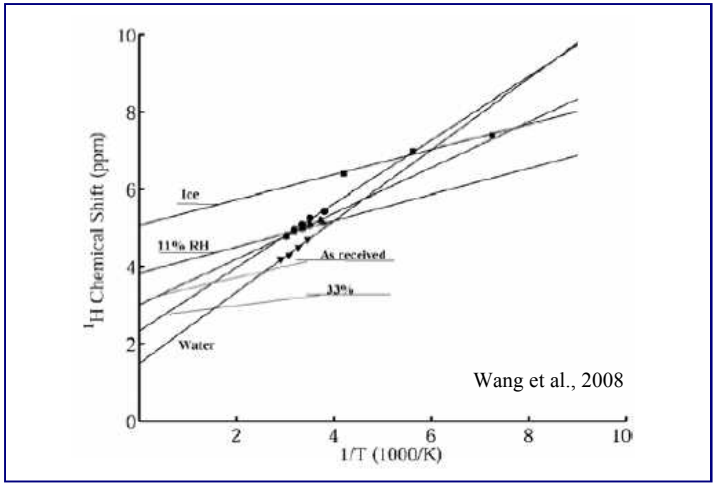
Wang et al., 2003, Mat. Res. Soc. Symp. Proc.; 2003, Geology

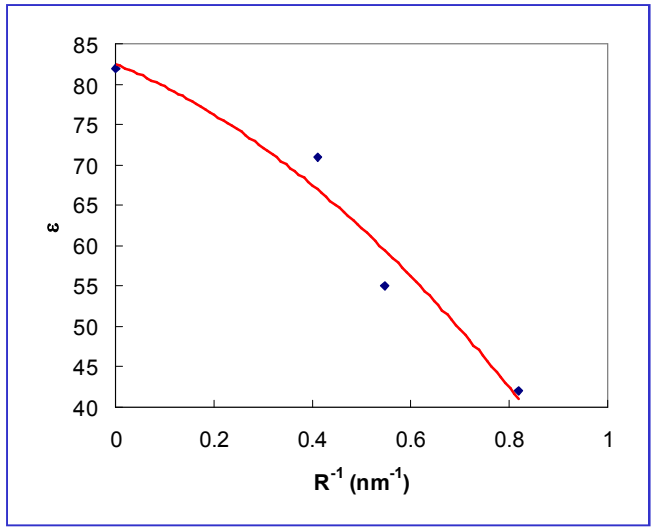
Sandia National Laboratories

Effect of Nanopore Confinement on Water



Kolesnikov et al., 2004





Senapati & Chandra, 2001, J. Phys. Chem.

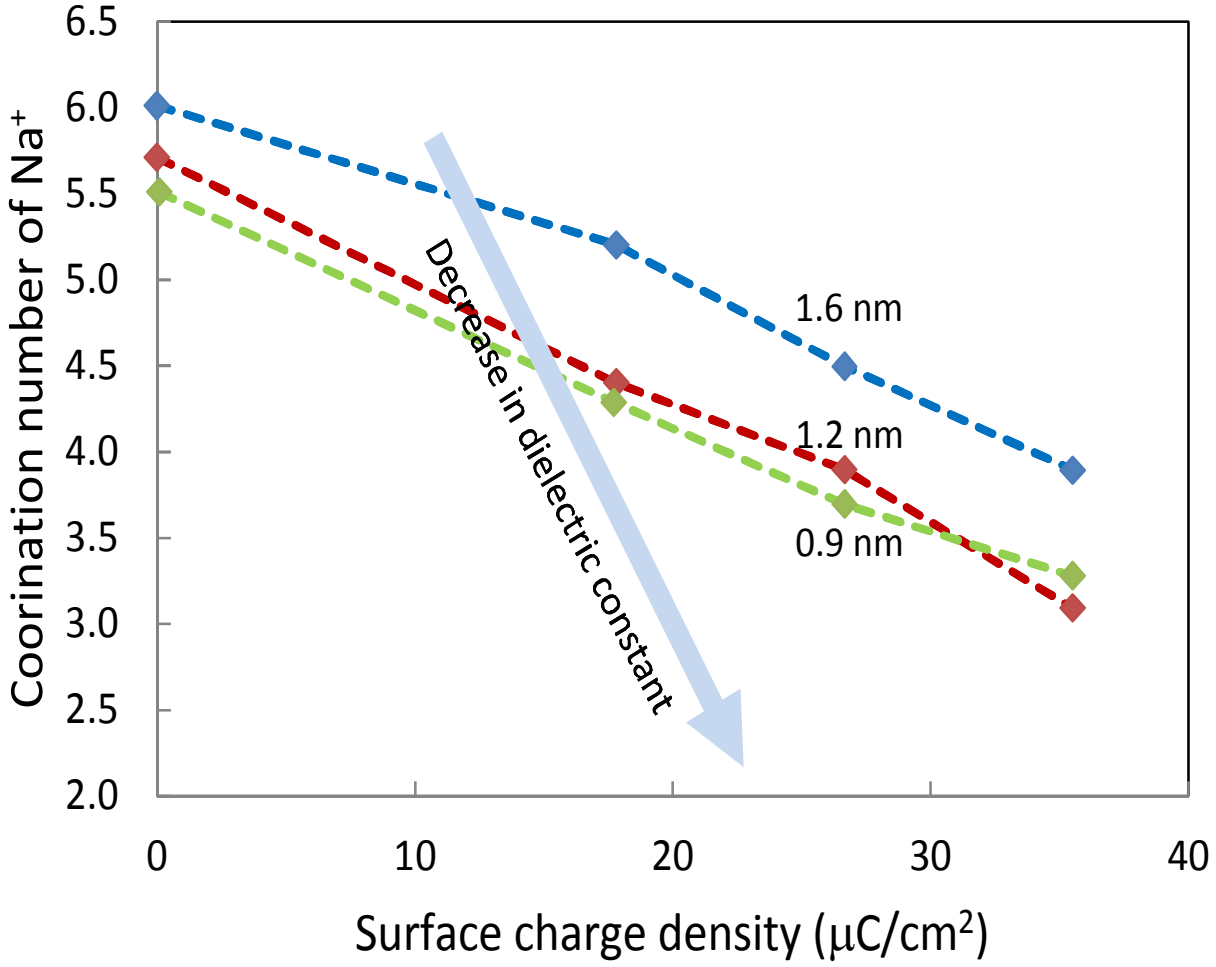
Postulations:

Water molecules in nanopores are more restrained.

$H_4SiO_4 = SiO_2(s) + 2H_2O$ pptn

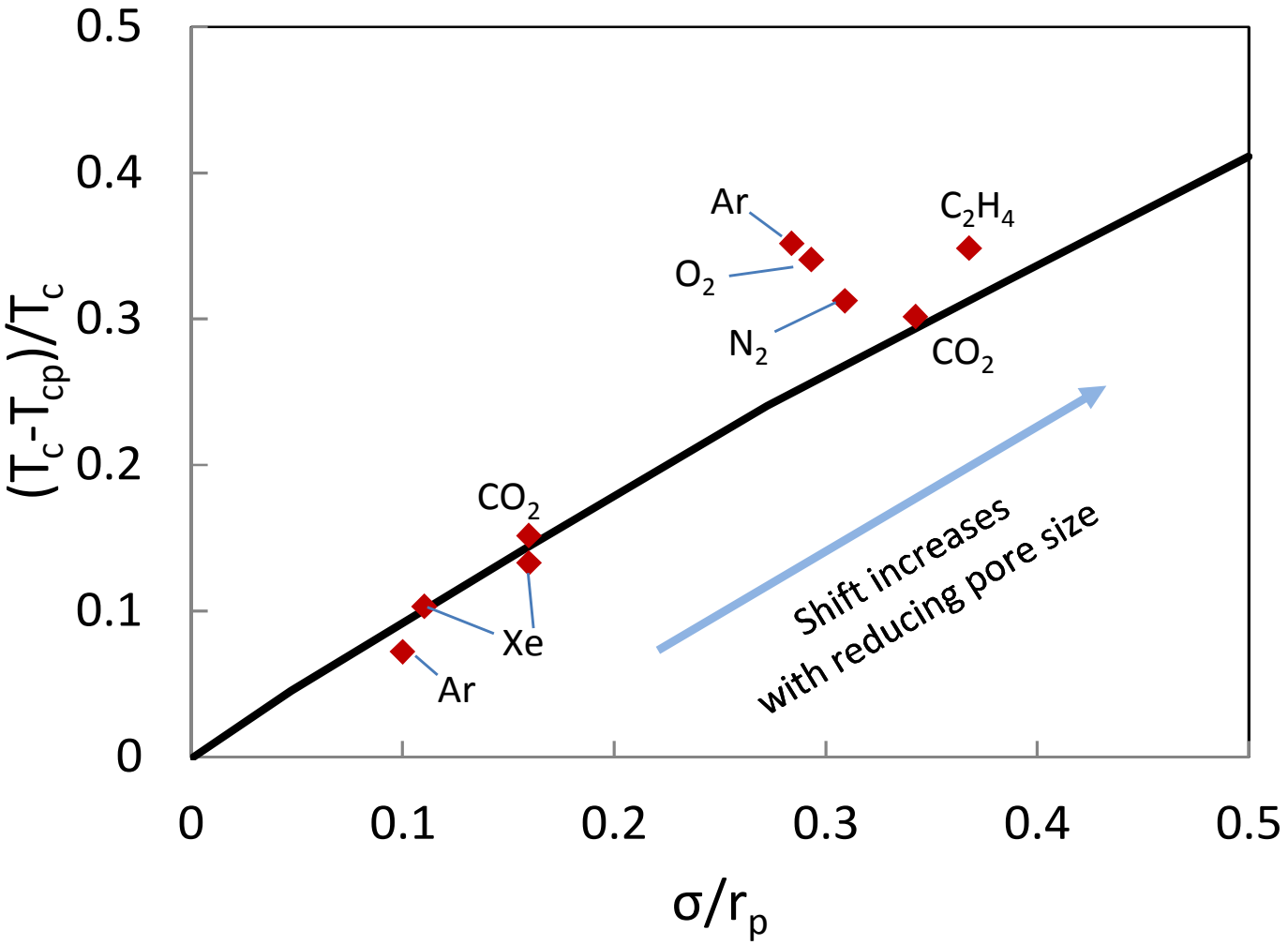
$M(H_2O)_n^{z+} = M^{z+} + nH_2O$ inner sphere

Sandia National Laboratories

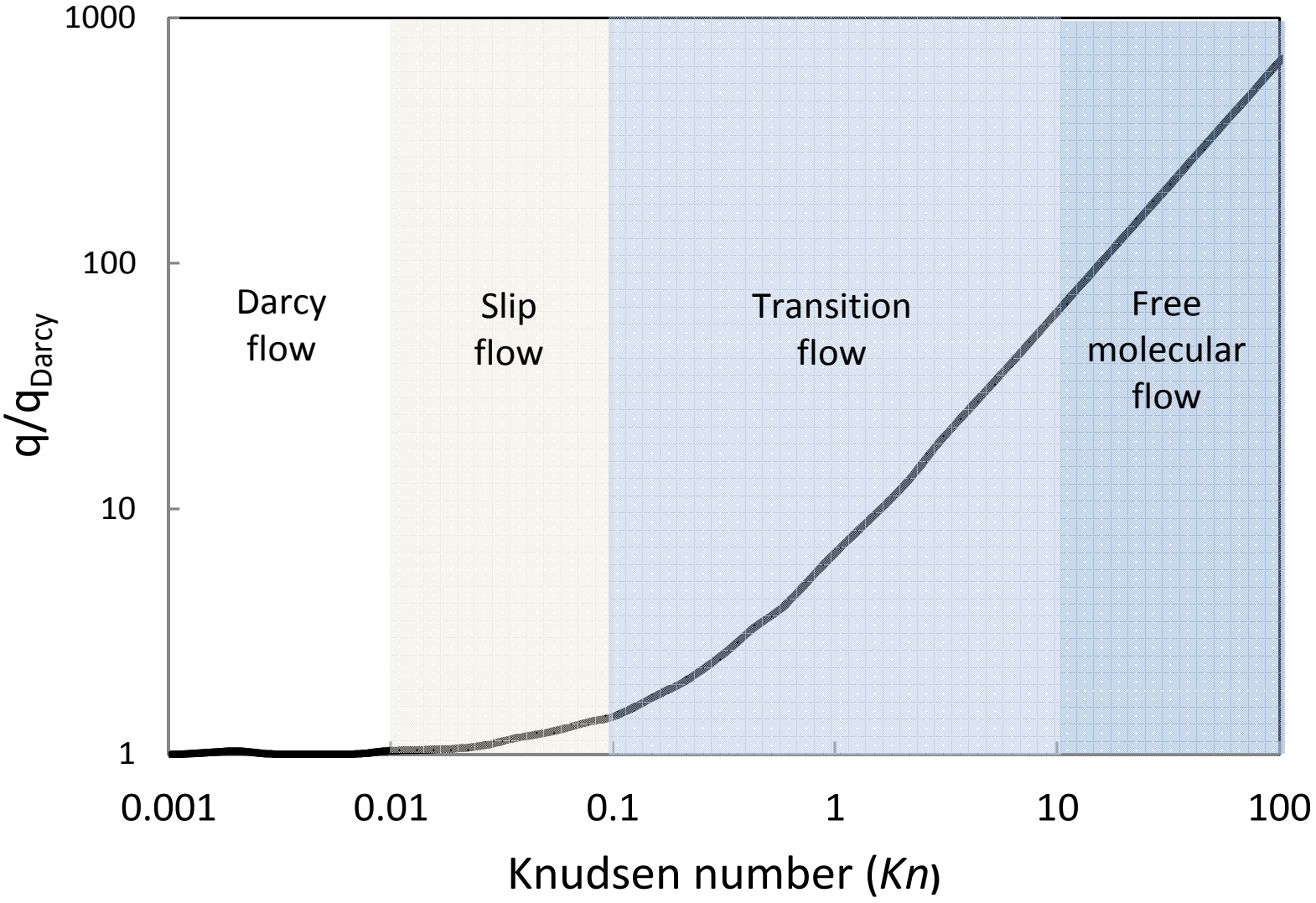


Kalluri et al. (2011).

Sandia National Laboratories

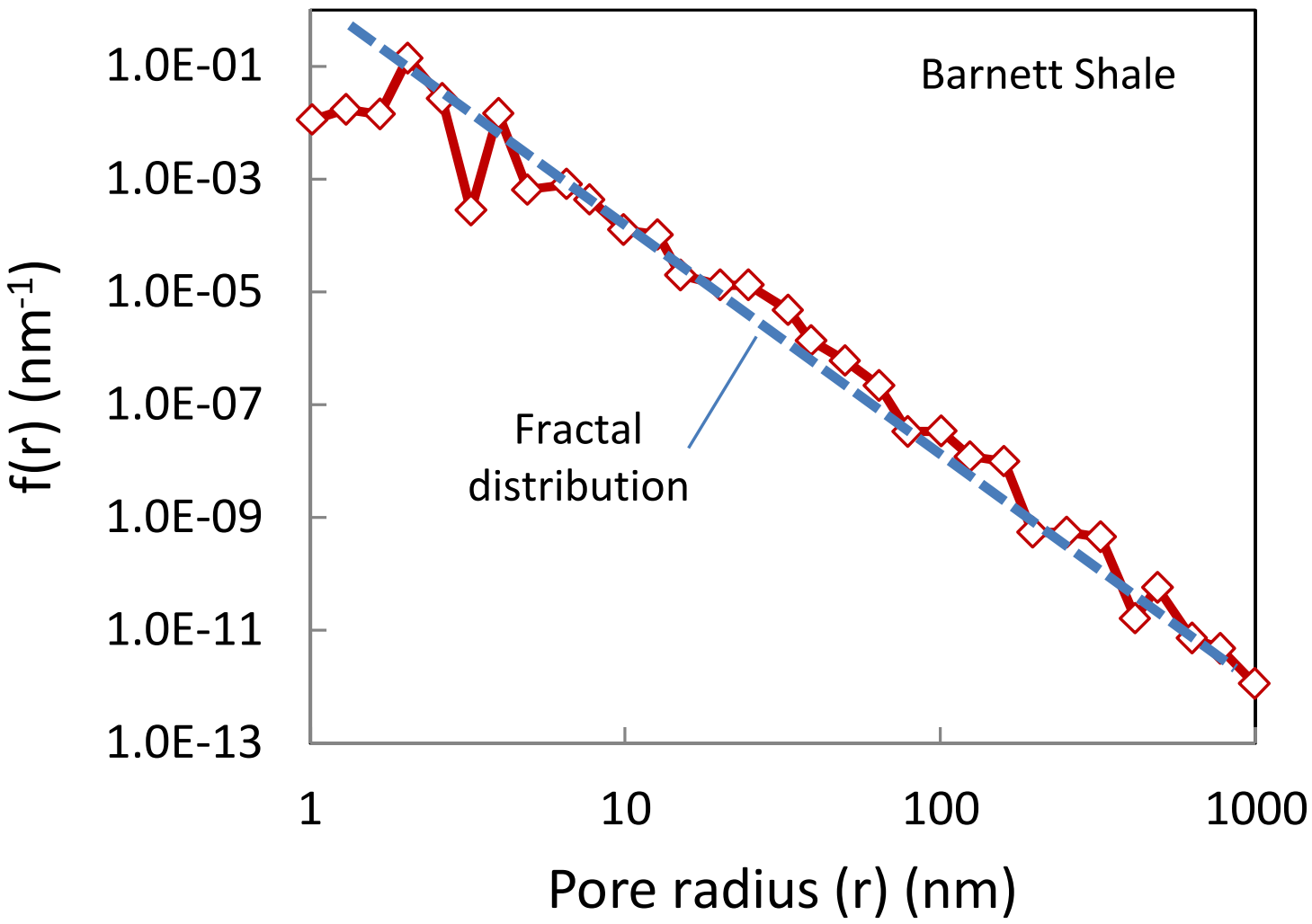


Sandia National Laboratories



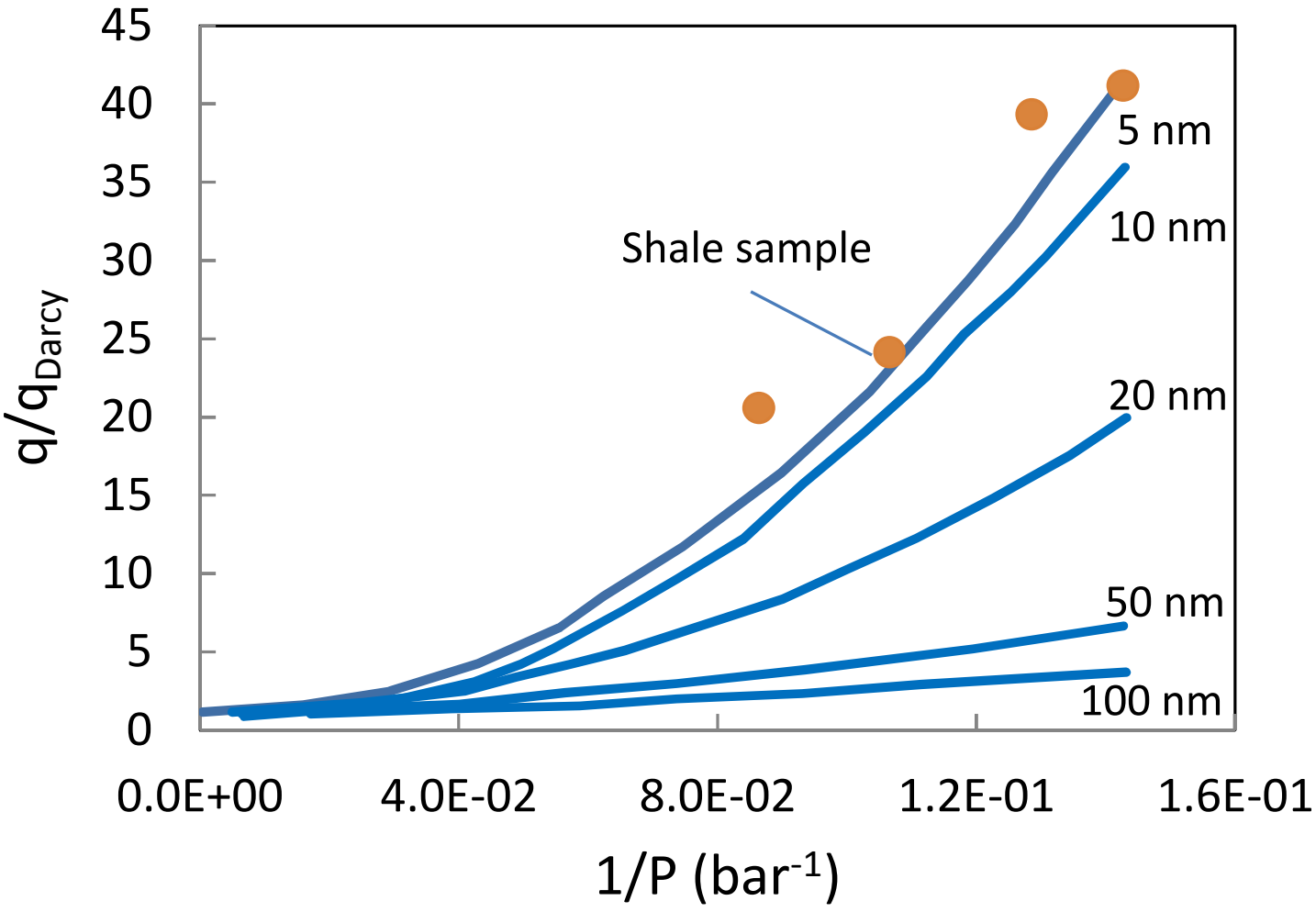
Ziarani and Aguilera (2012)

Sandia National Laboratories



Clarkson et al. (2012)

Sandia National Laboratories

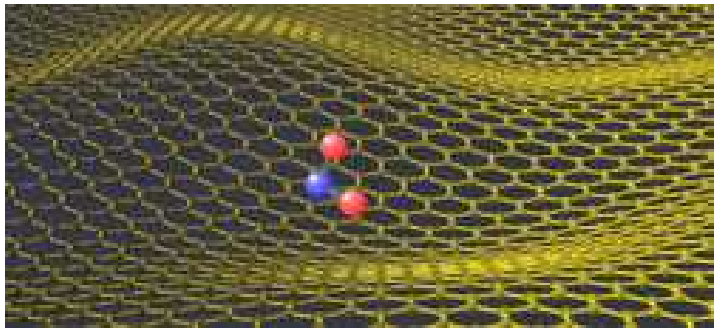


Fathi et al. (2012)

Sandia National Laboratories

Concluding Remarks

- Size matters!
  - Novel mineral-fluid interface chemistry may emerge when the dimension of one of the phases is reduced to nanometers.
- Texture matters!
  - Measurements on “isolated”, unconfined surfaces may not be representative of actual geologic materials.
- Perspectives
  - Progress in nanoscience & technology
  - Emergence of new properties through cooperative processes
- Geochemical implications (Wang et al., 2011, in Frontier in Geochemistry)
  - New perspectives for understanding fundamental geochemical processes
  - Development of novel materials for environmental applications



Graphene sensor

(Hadlington, 2008)

Acknowledgments

Contributors:

A. Miller (Sandia)

H. Gao (Former Sandian)

Ed Matteo (Sandia)

J. Kruichak (Sandia)

C. Bryan (Sandia)

J. Brinker (Sandia)

H. Xu (Univ. of Wisconsin)

Funding sources:

Sandia is multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Co., for the United States Department of Energy (US DOE) under Contract DE-AC04-94AL8500. This research is supported by DOE LDRD program, DOE OCRWM S&T Program, DOE-UFD program, and the National Science Foundation.

Sandia National Laboratories