Water sorption in nanoporous silica via molecular simulations

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Porous Materials in cars

Sensors (e.g., ensure an optimum engine combustion)[1,2]

http://www.autoevolution.com

Gas capture (e.g., catalytic converter to reduce greenhouse gas emissions)[1,2]

[1] D. J. Wales et al. *Chem. Soc. Rev.* 44 (2015) 4290
[2] T. Wagner et al. *Chem. Soc. Rev.* 42 (2013) 4036

Porous Materials Design

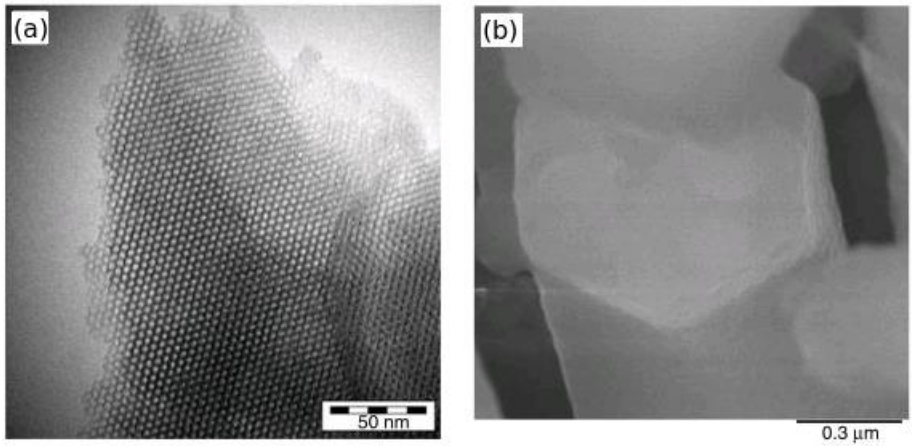
Reduce cost: use cheap and robust porous materials

(e.g., reduce the use of precious, expensive materials (Platinum, Palladium, Rhodium, …) like in catalytic converters)

Silica (Zeolites, mesoporous silica (e.g., MCM-41, SBA-15))

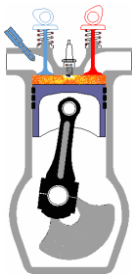
Transmission Electron Microscopy (TEM) image of MCM-41

Schreiber et al., Phys. Chem. Chem. Phys. , 3 (2001) 1185



Hydrophilic materials

Sensor for monitoring the amount of water vapor



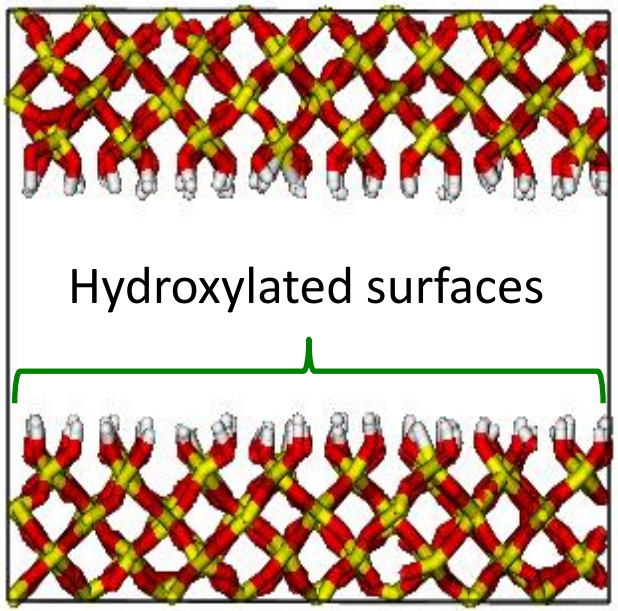
Ideal internal combustion in engines:

Hydrocarbons + O_2 → H_2O + CO_2

Molecular simulations and models

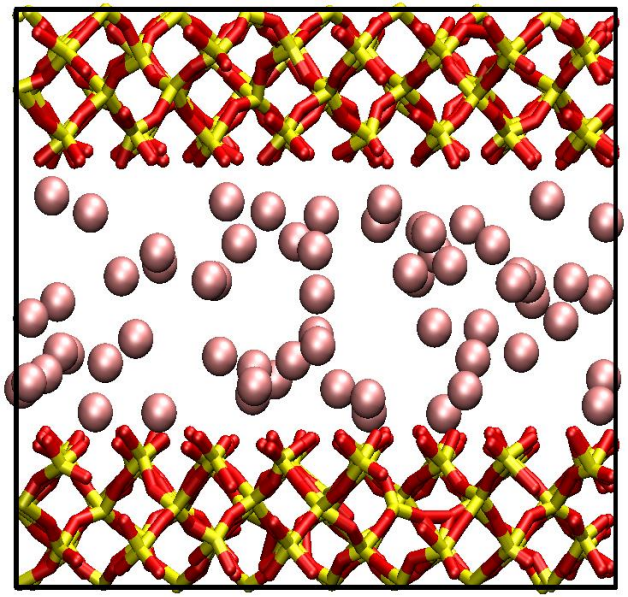
2 molecular models (effect of surface chemistry)

SiO_2-OH



7.8 $OH.nm^{-2}$

SiO_2-Cs^+

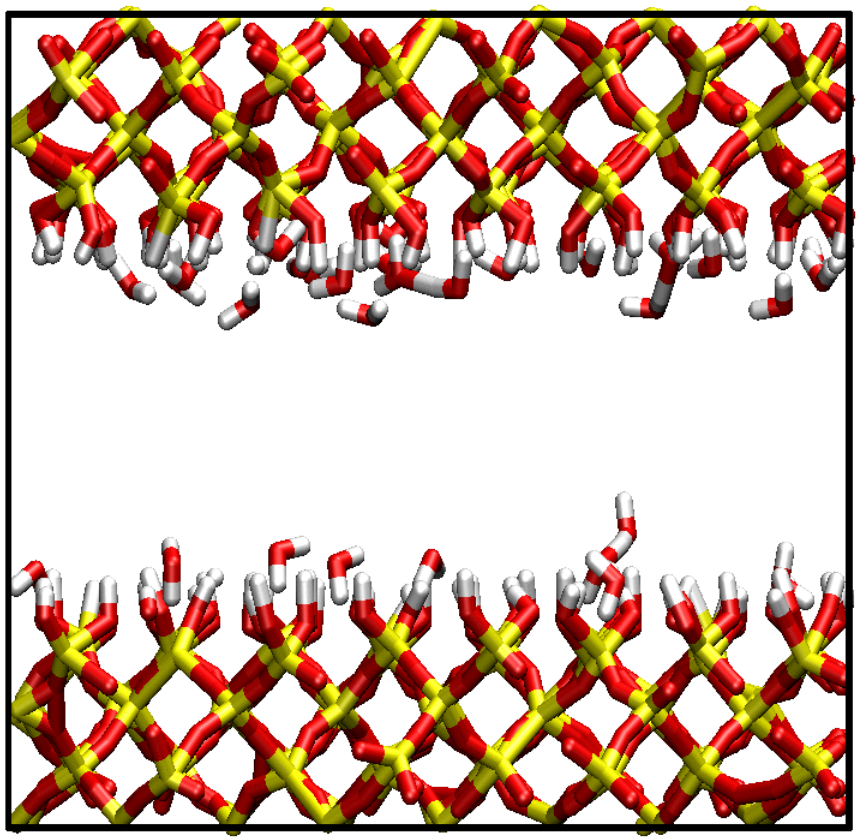


$\sigma \sim -0.6\ C.m^{-2}$

+ Grand canonical Monte Carlo to simulate water sorption isotherms

Pictures of water sorption mechanisms

SiO_2-OH



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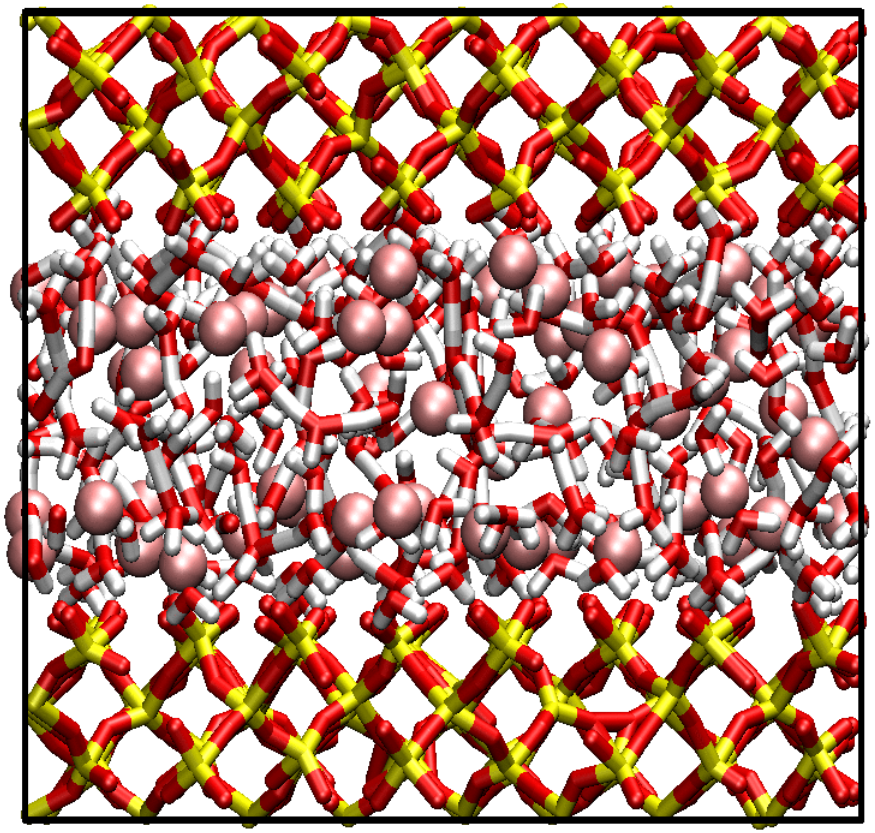
SiO_2-Cs^+



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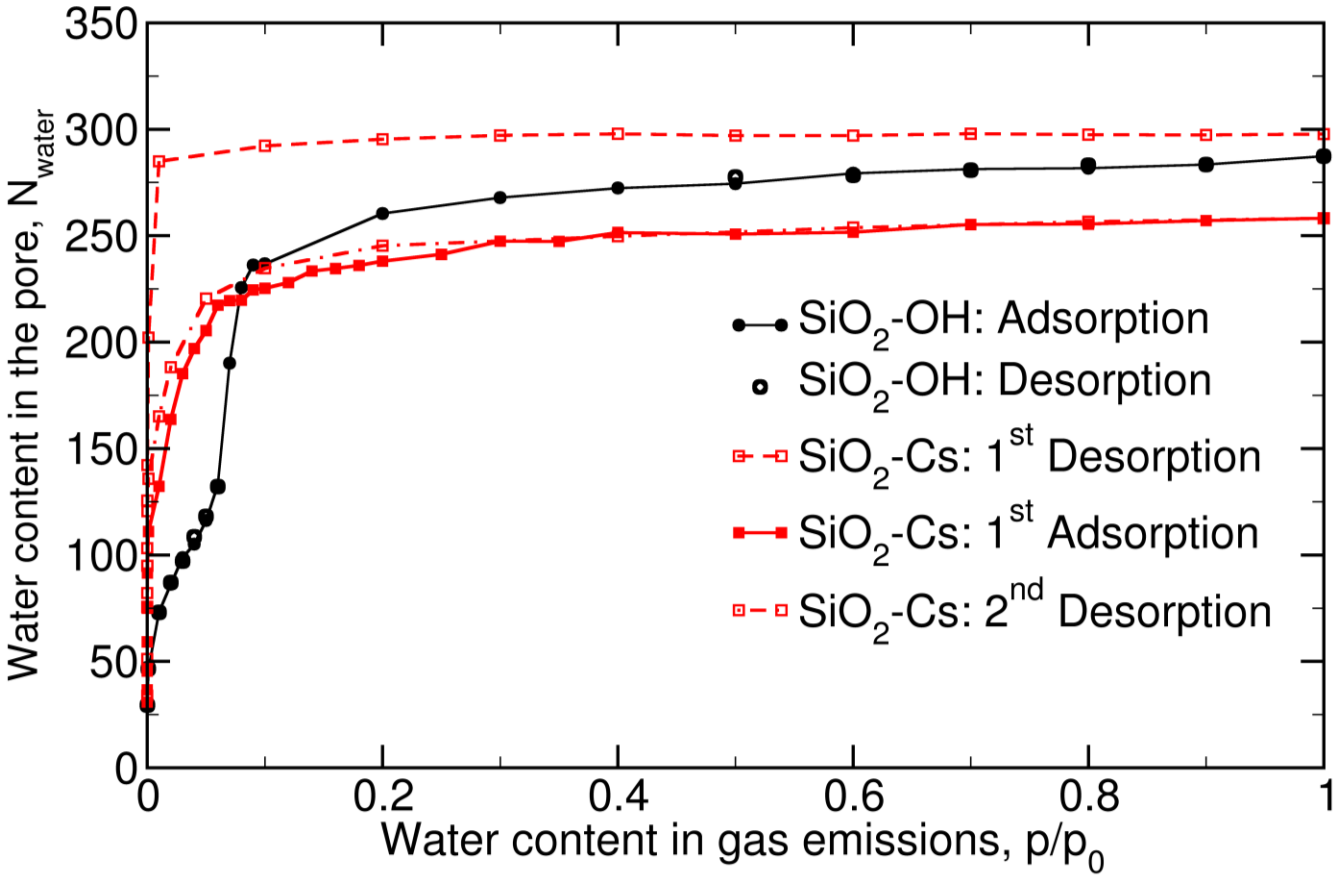
Water sorption isotherms



We can relate the water content within the pore with the water content of car gas emissions **(combustion efficiency)**

Summary

- Nanoporous silica is a good candidate for the design of sensors in car industry
- We explored different surface states (chemistry) in silica nanopores in order to observe the effect on water sorption
- The structure of bi-component confined fluids (water and Cs^+ counterions) affects water sorption properties