Abstract Submitted
for the DFD17 Meeting of
The American Physical Society

Numerical analyses on the effect of capillary condensation on gas diffusivities in porous media YUTA YOSHIMOTO, TAKUMA HORI, IKUYA KINEFUCHI, SHU TAKAGI, The University of Tokyo — We investigate the effect of capillary condensation on gas diffusivities in porous media composed of randomly packed spheres with moderate wettability. Lattice density functional theory simulations successfully reproduce realistic adsorption/desorption isotherms and provide fluid density distributions inside the porous media. We find that capillary condensations lead to the occlusion of narrow pores because they preferentially occur at confined spaces surrounded by the solid walls. Consequently, the characteristic lengths of the partially wet structures are larger than those of the corresponding dry structures with the same porosities. Subsequent gas diffusion simulations exploiting the mean-square displacement method indicate that while effective diffusion coefficients significantly decrease in the presence of partially condensed liquids, they are larger than those in the dry structures with the same porosities. Most importantly, we find that the porosity-to-tortuosity ratio, which is a crucial parameter that determines the effective diffusion coefficient, can be reasonably related to the porosity even for the partially wet porous media.

Yuta Yoshimoto
The University of Tokyo

Date submitted: 01 Aug 2017 Electronic form version 1.4