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Percolation and diffusion in two dimensional random media
BONG JUNE SUNG, ARUN YETHIRAJ, Department of Chemistry, University of Wisconsin-Madison — The diffusion of hard disc fluids in two dimensional porous media (composed of immobile hard discs) is studied using discontinuous molecular dynamics (DMD) simulations and analyzed using a Voronoi tessellation procedure. A pore is defined as a circle tangential to three neighbor matrix discs with a pore center at a Voronoi vertex. If an edge of Voronoi diagram connecting two pores is too narrow for a fluid particle to move along, the edge is considered disconnected. This procedure maps the system onto a lattice model with diffusion possible in the bond percolation limit. The percolation threshold, p_c of edges connecting pores is found to be 0.526, where p is the fraction of connected edges. p_c is significantly different from $p_r = 2/3$ of random bond percolation theory where the edge connectivity of the same Voronoi diagram is determined randomly. This suggests that the edge connectivity is strongly correlated even for randomly distributed medium particles. DMD simulations show normal diffusion for $p > p_r$, confined dynamics for $p < p_c$, and anomalous diffusion for $p_c < p < p_r$.

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