Molecular simulation of nitrogen adsorption in nanoporous silica

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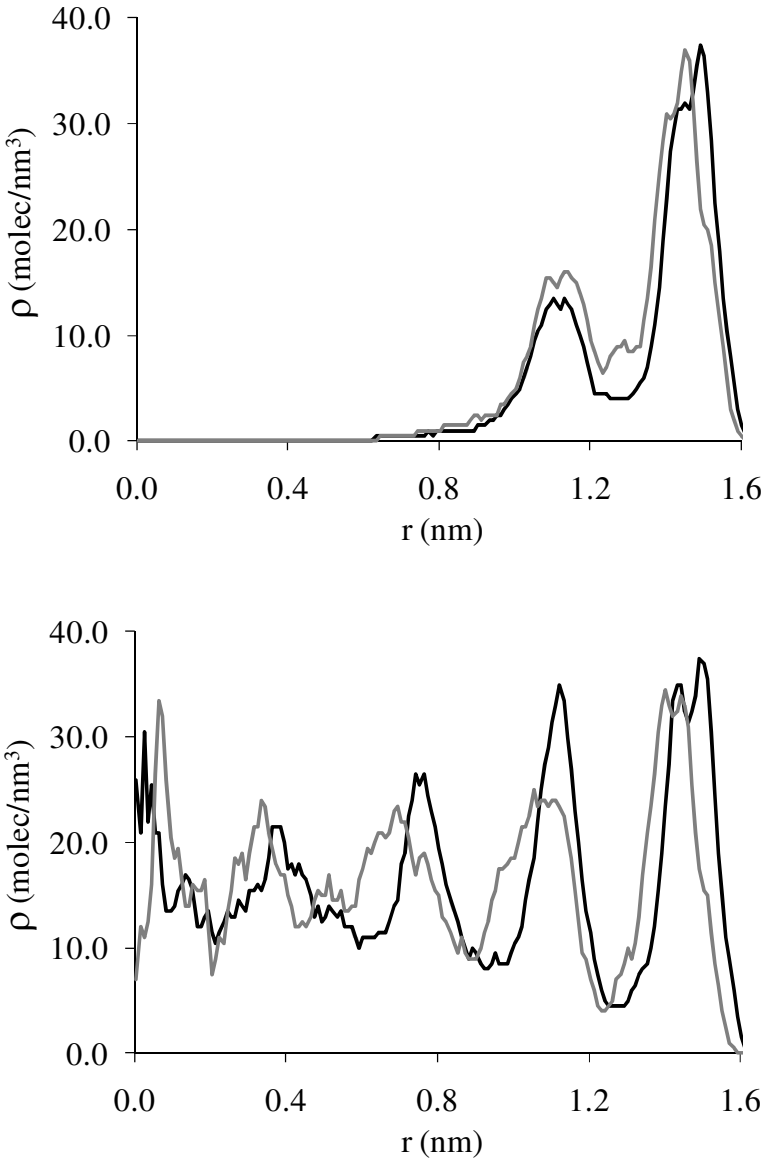

Figure S1. (top) Density profiles ρ(r) for nitrogen confined at 77 K in the silica cylindrical nanopore with D = 3.2 nm at the onset of capillary condensation: (black line) pea model, (grey line) bean model. r = 0 corresponds to the pore center. (bottom) same as top but at a pressure above capillary condensation.

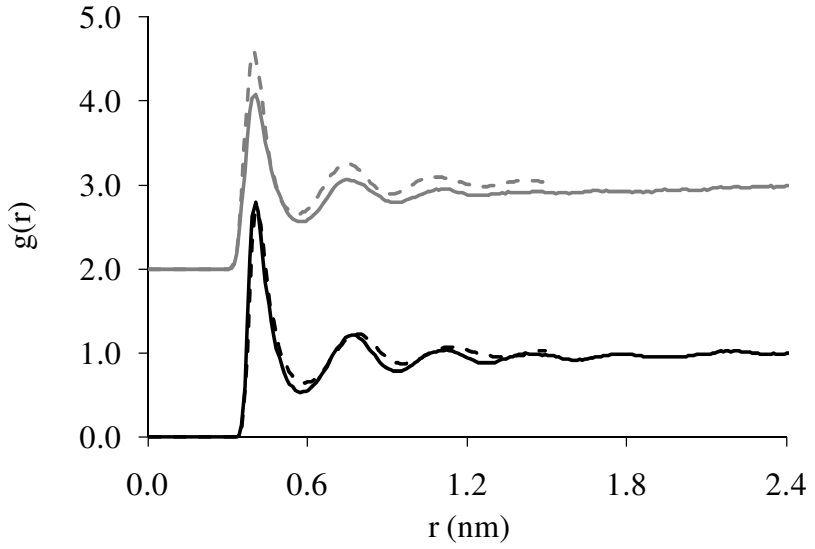

Figure S2 Pair correlation function g(r) for nitrogen confined at 77 K after capillary condensation in the silica cylindrical nanopore with D = 3.2 nm: (black lines) pea model, (grey lines) bean model. The solid lines are for the confined fluid while the dashed lines are for the bulk fluid. The pair correlation functions for the bean model have been shifted up by +2 for the sake of clarity. All the pair correlation functions for the confined fluid have been corrected for excluded volume effect.

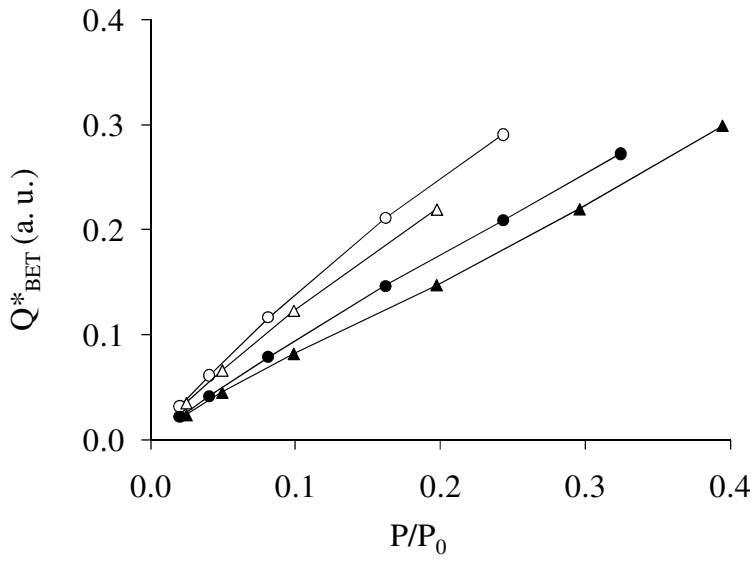

Figure S3. BET plots for nitrogen adsorption at 77 K in silica cylindrical nanopores. $Q^* = \frac{P/P_0}{N(1-P/P_0)}$ is the left handside of the BET equation. (circles) pea model and (triangles) bean model. Open and closed symbols correspond to the pores with D = 3.2 nm and D = 4.8 nm, respectively. Following the work by Kruk et al.,[Error! Bookmark not defined.] the linear range of data between 0.04 and 0.2 P_0 was considered for each plot to estimate the BET surface as well as the C_{BET} parameter.