Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

The role of the potential field on occurrence and flow of octane in quartz nanopores

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Supplementary Figures

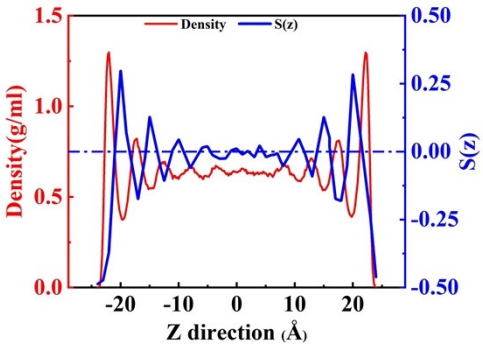

Fig. S1. Profiles of density (red line) and the orientation order parameter (blue line), $S(z) = 1.5\langle\cos^2\theta(z)\rangle$-0.5, where θ is the angle between the straight line connecting the two carbon atoms at the end of an octane molecule and the normal vector to the silica surface, the angular brackets denote an average.

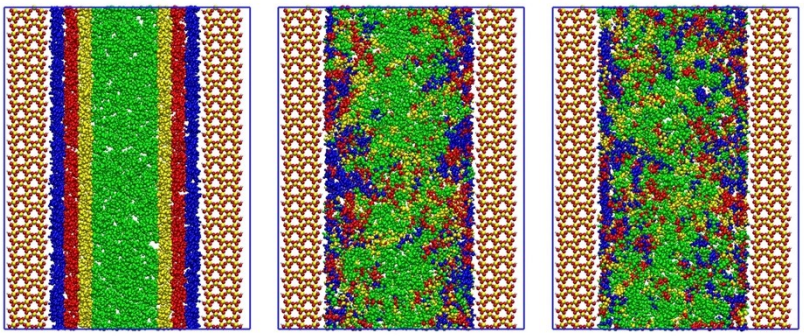

Fig. S2. Representative snapshots of octane molecules at 5.0, 5.1, and 5.2 ns, in the w = 50 Å nanopore. For clarity, the molecules at 5.0 ns, in the first, second and third adsorption layers, are highlighted in blue, red and yellow, respectively.

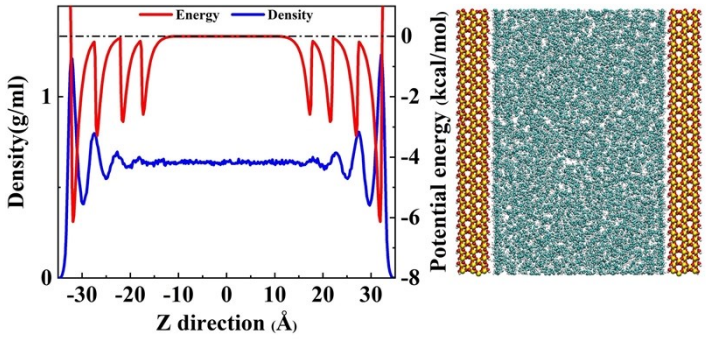

Fig. S3. Density profile (blue line), potential energy profile (red line) and the snapshot of octane in the nanopore with w = 70 Å.

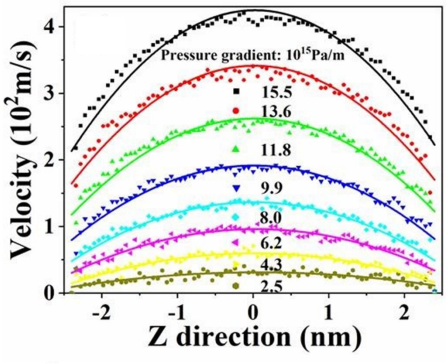

Fig. S4. Velocity profiles of octane at different external pressure gradients in the w = 50 Å nanopore.

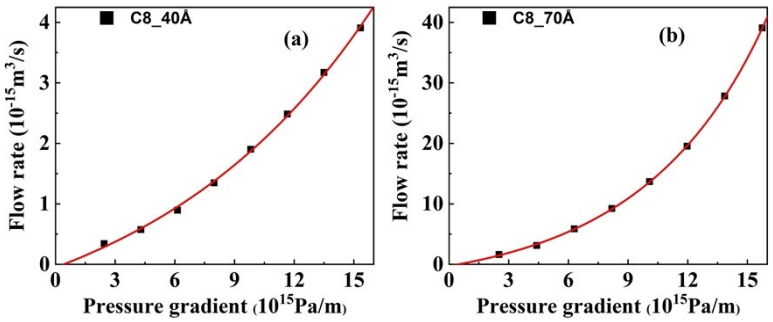

Fig. S5. Dependence of octane flow rate on external pressure gradients in (a) w = 40 Å and (b) w = 70 Å nanopores.