Describing binary mixture diffusion in carbon nanotubes with the Maxwell-Stefan equations. An investigation using molecular dynamics simulations

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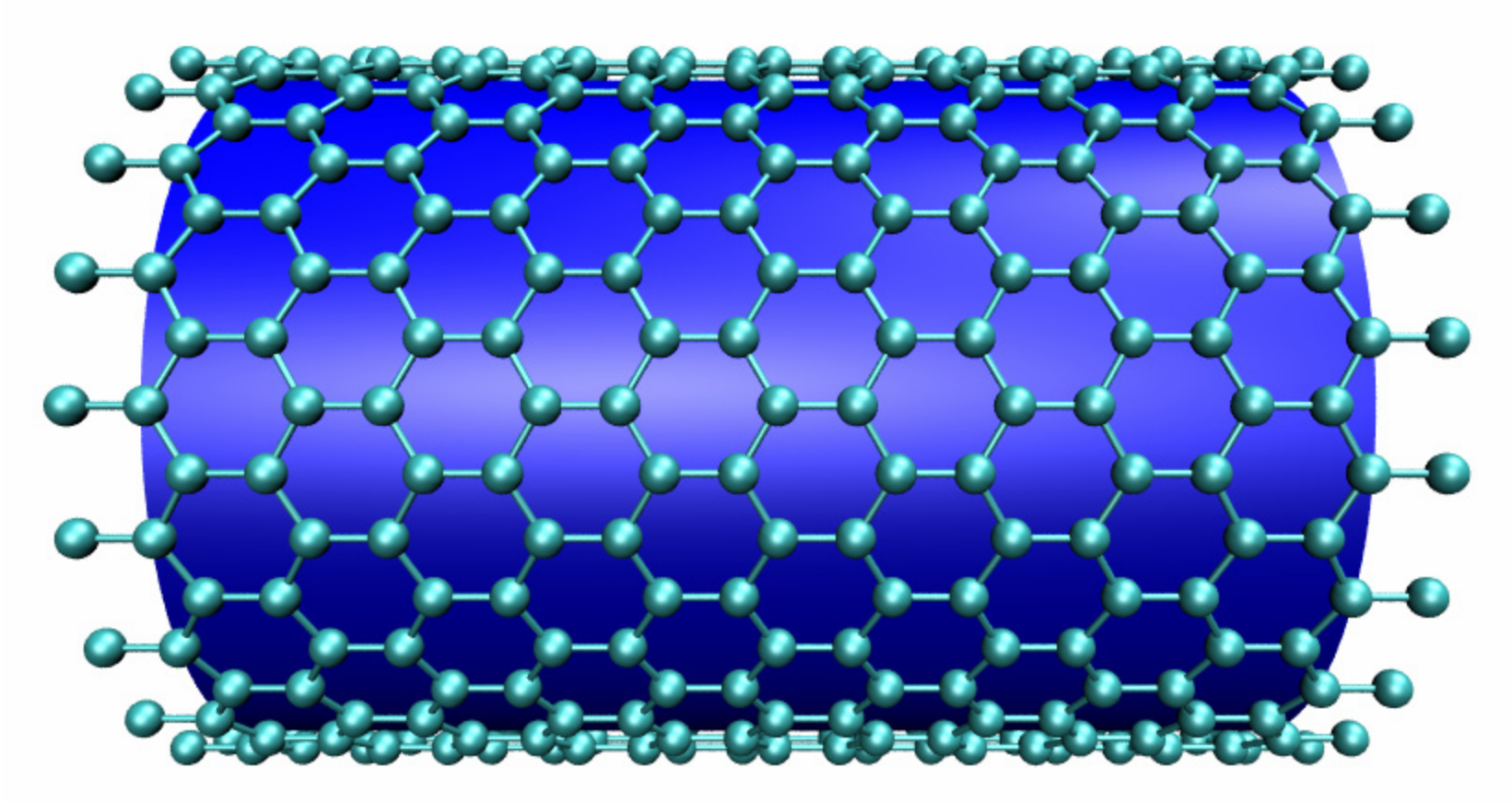
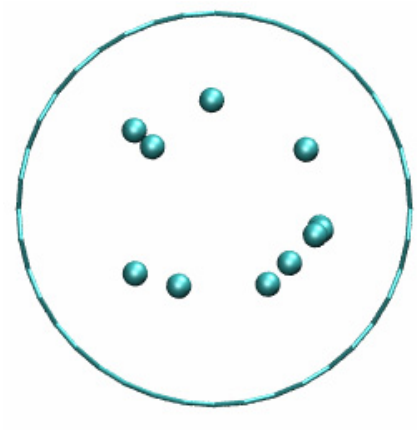
- Contains data on Δ_{ij}, $D_{i,self}$, $Đ_i$, $Đ_{ii}$ for all the campaigns listed in Table 1 of the manuscript
- The symbols represent the MD simulated data
- The continuous solid lines represent calculations based on the Maxwell-Stefan theory, Eqs (14) and (15), and using pure component parameters listed in Table 4.

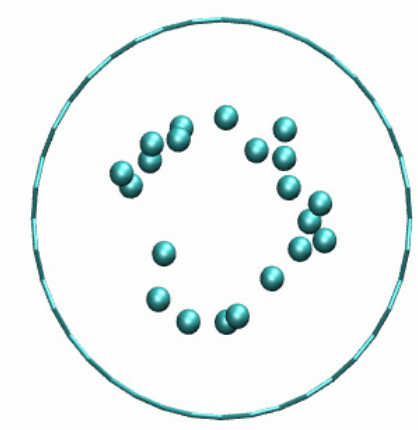
CNT (20,0)



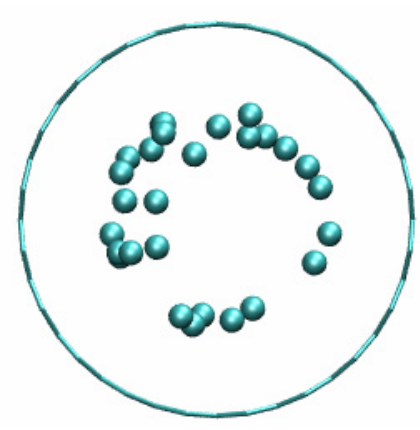
CNT (20,0); pure C1 adsorption, snapshots, 300 K



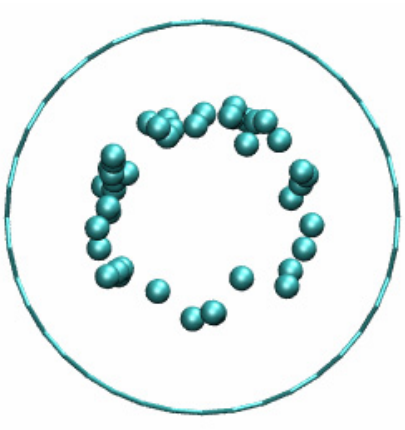
50 kPa



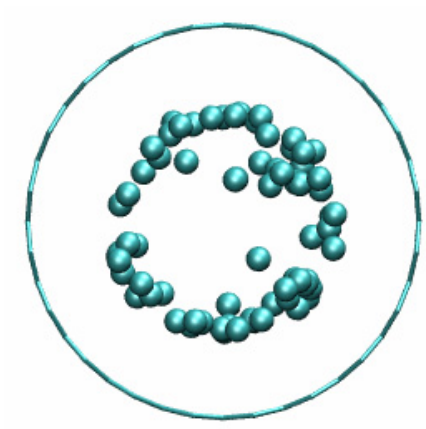
100 kPa



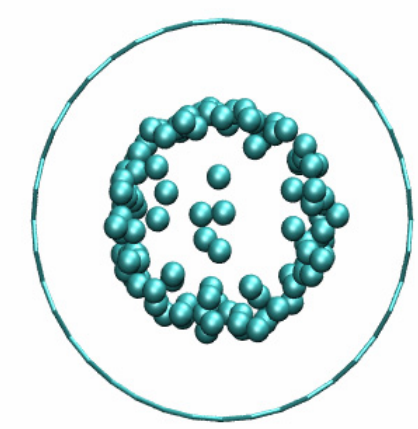
200 kPa



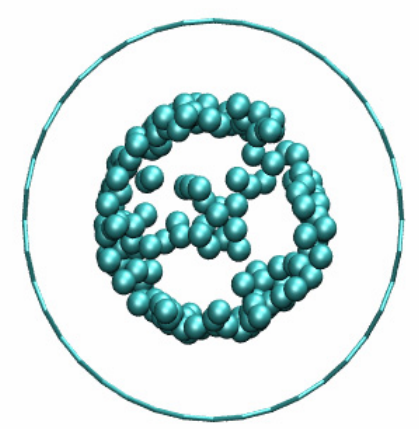
240 kPa



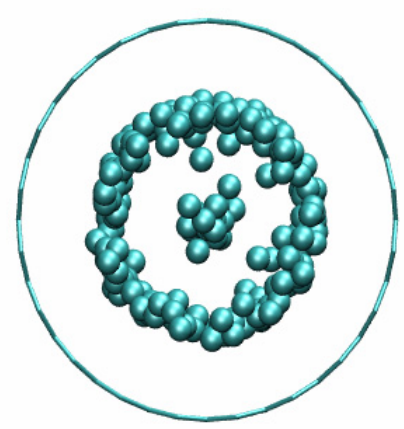
500 kPa



1000 kPa

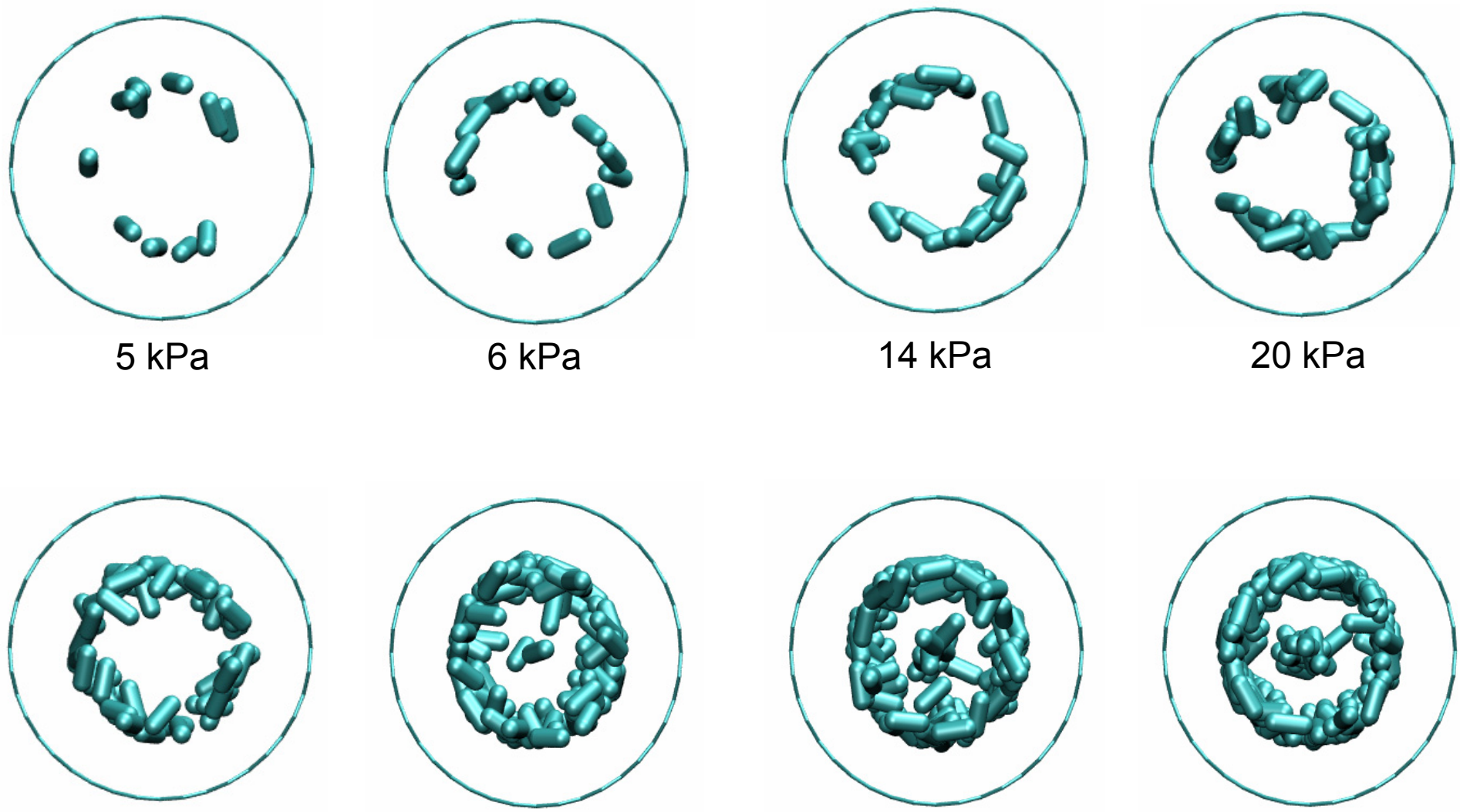


10000 kPa

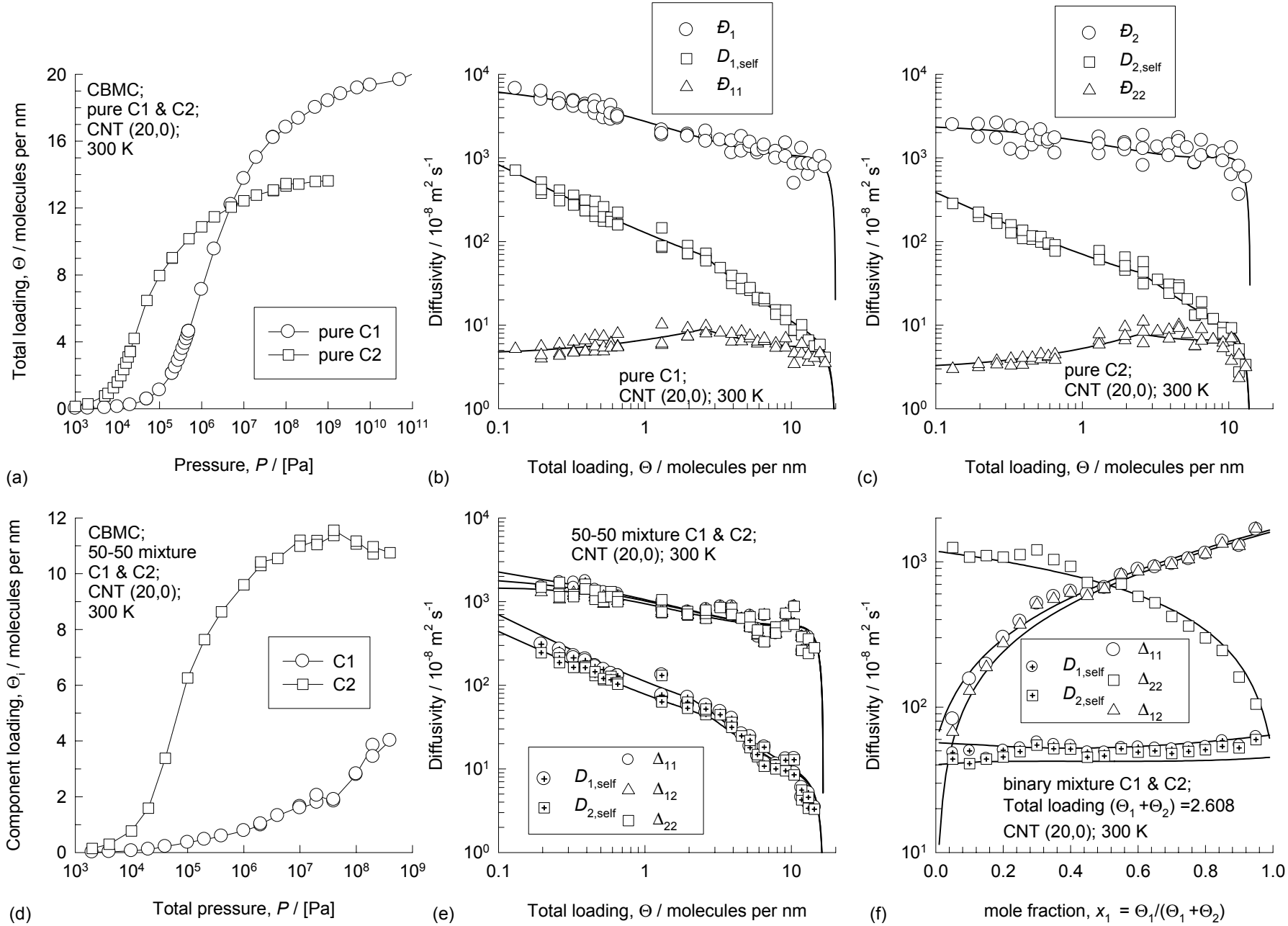


100000 kPa

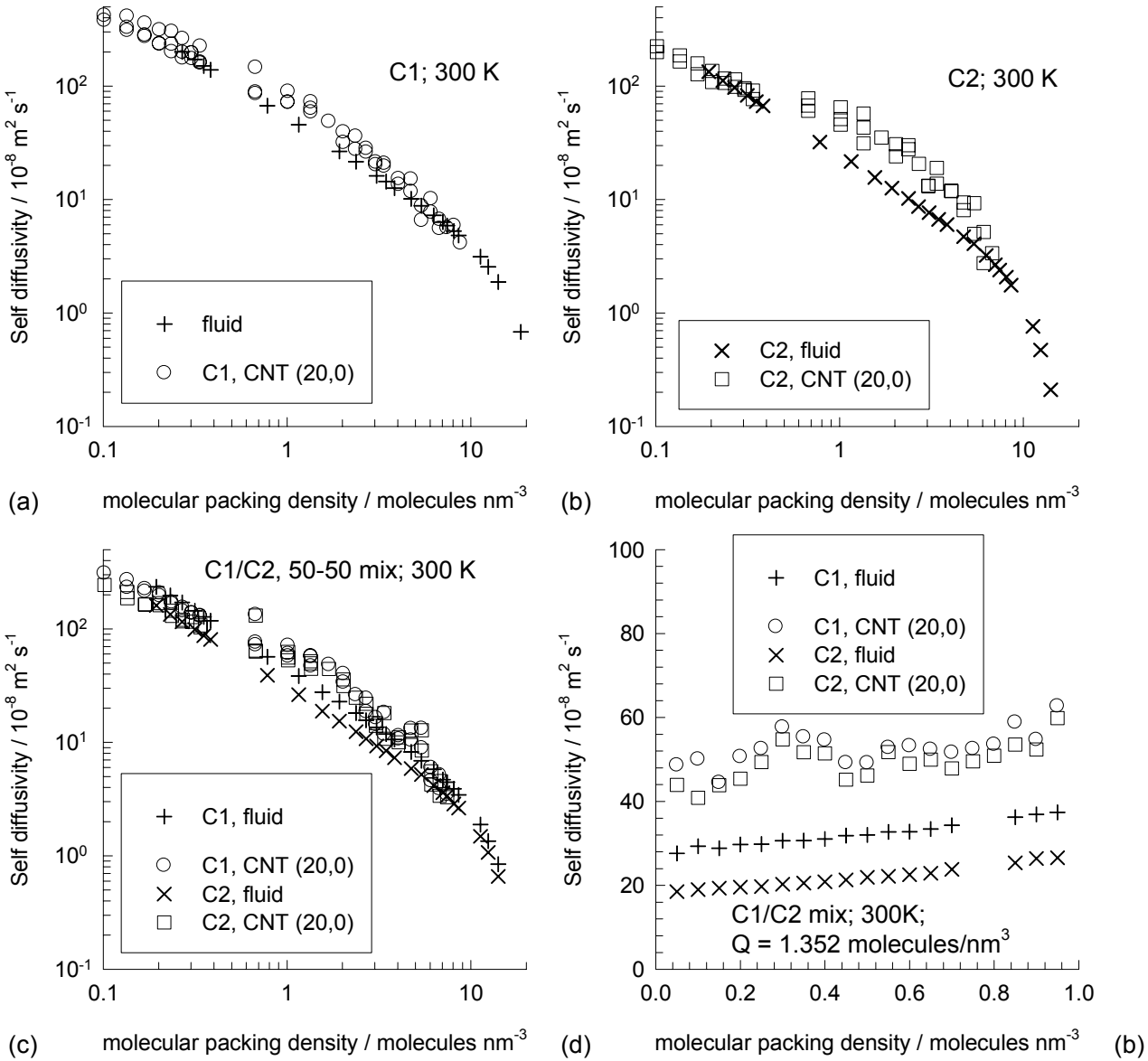
CNT (20,0); pure C2 adsorption, snapshots, 300 K



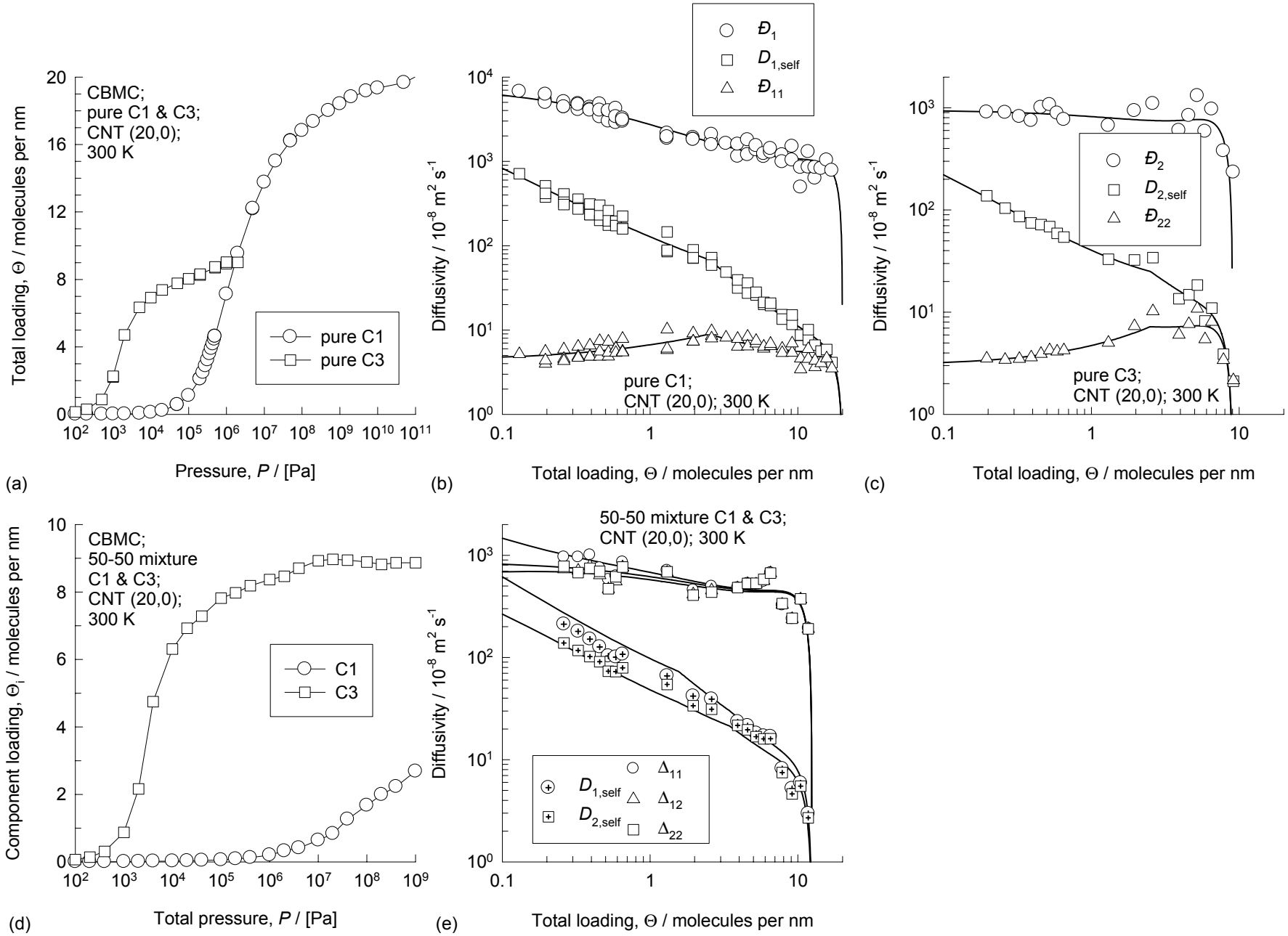
CNT (20,0); C1, C2, and C1-C2 mixture, 300 K



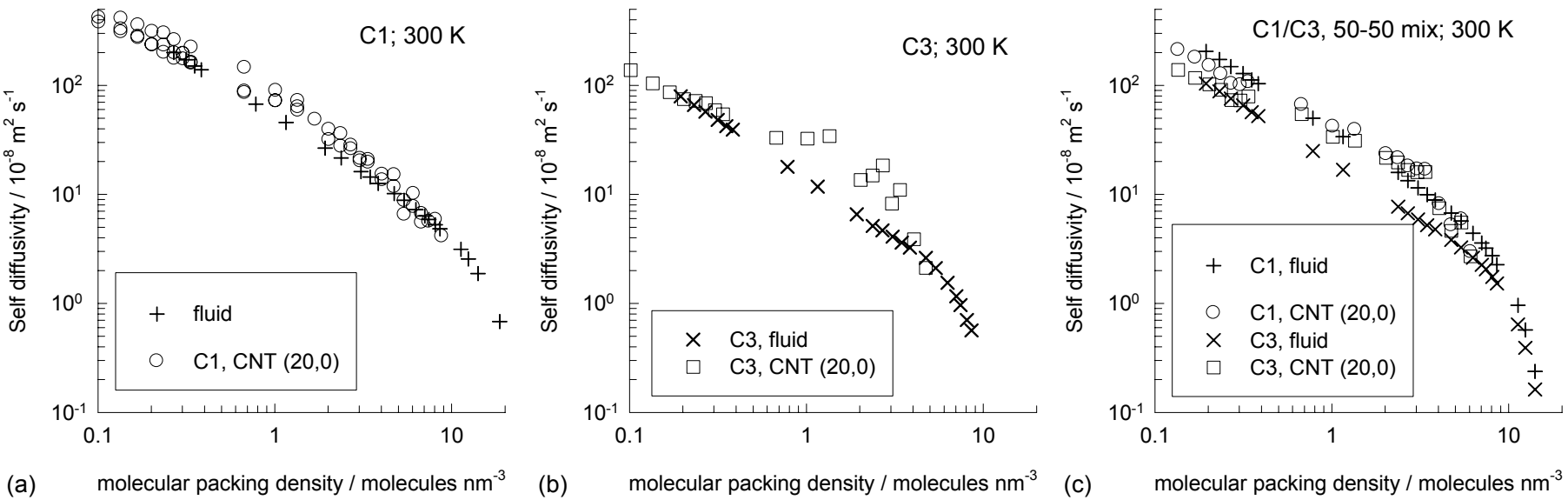
CNT (20,0) vs Fluid; C1, C2, and C1-C2 mixture, 300 K



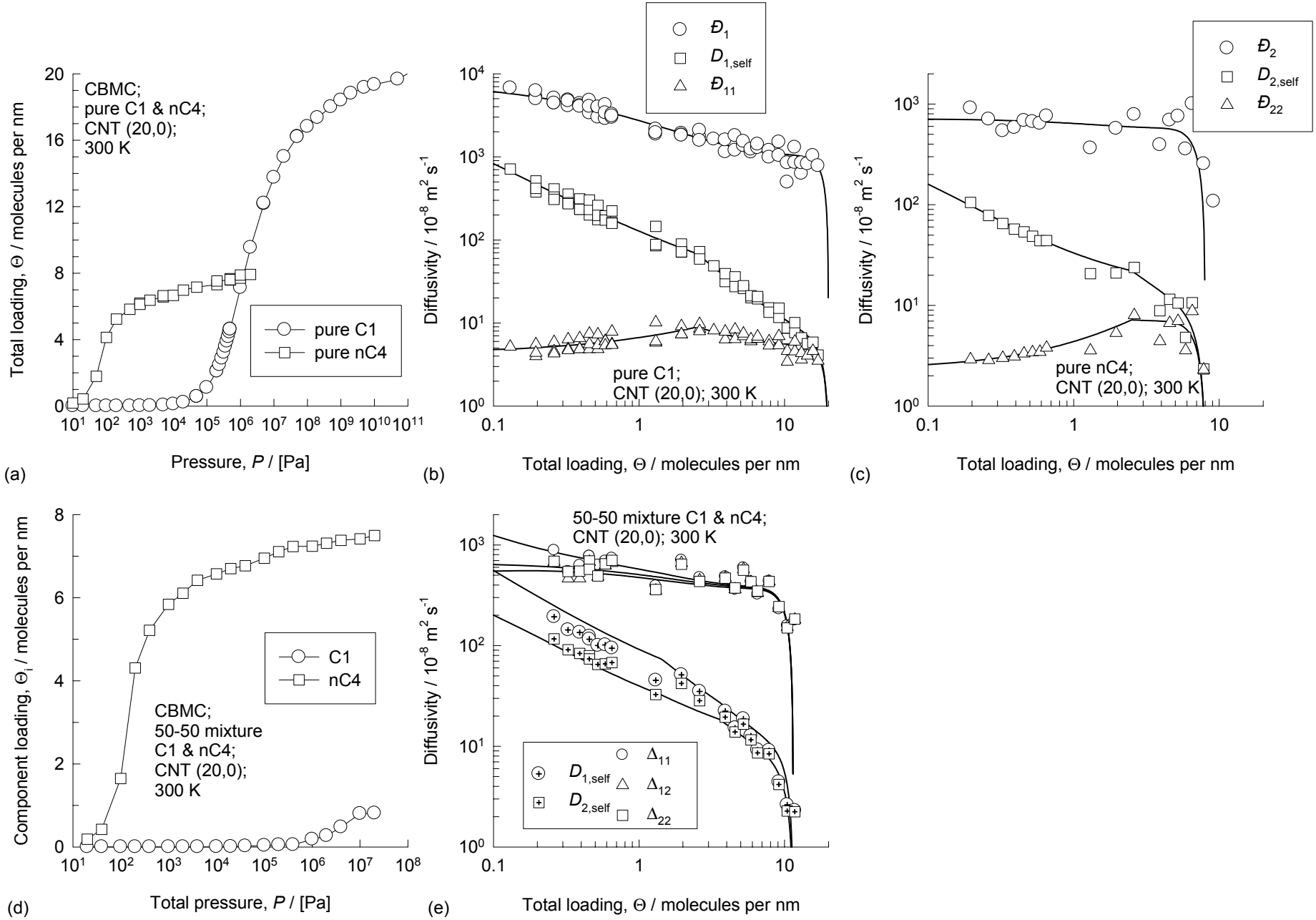
CNT (20,0); C1, C3, and C1-C3 mixture, 300 K



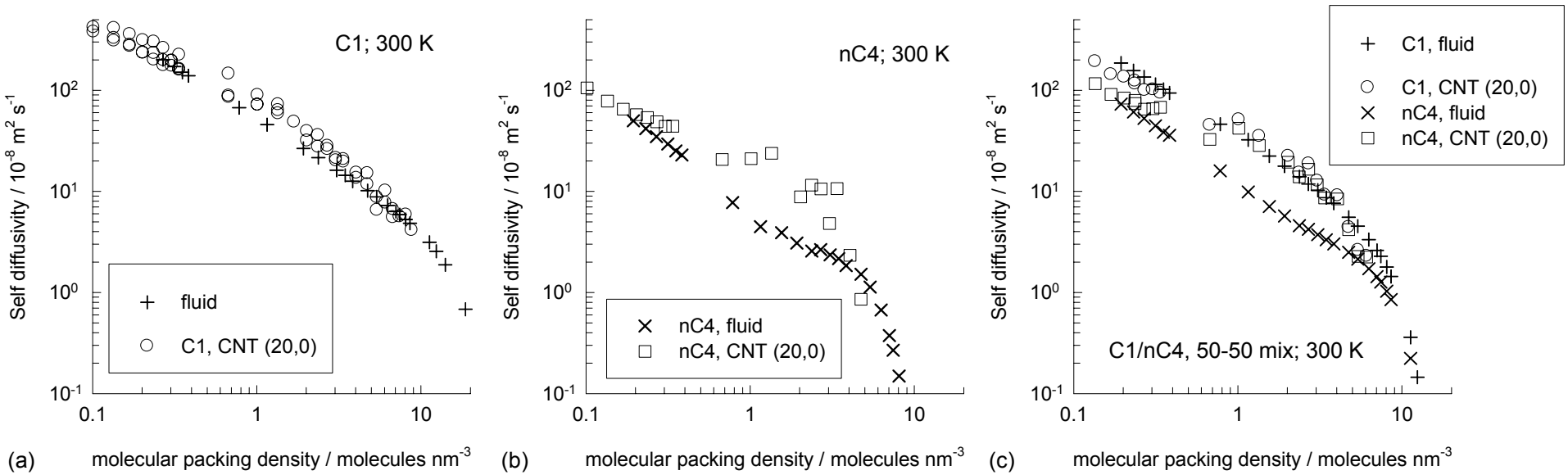
CNT (20,0) vs Fluid; C1, C3, and C1-C3 mixture, 300 K



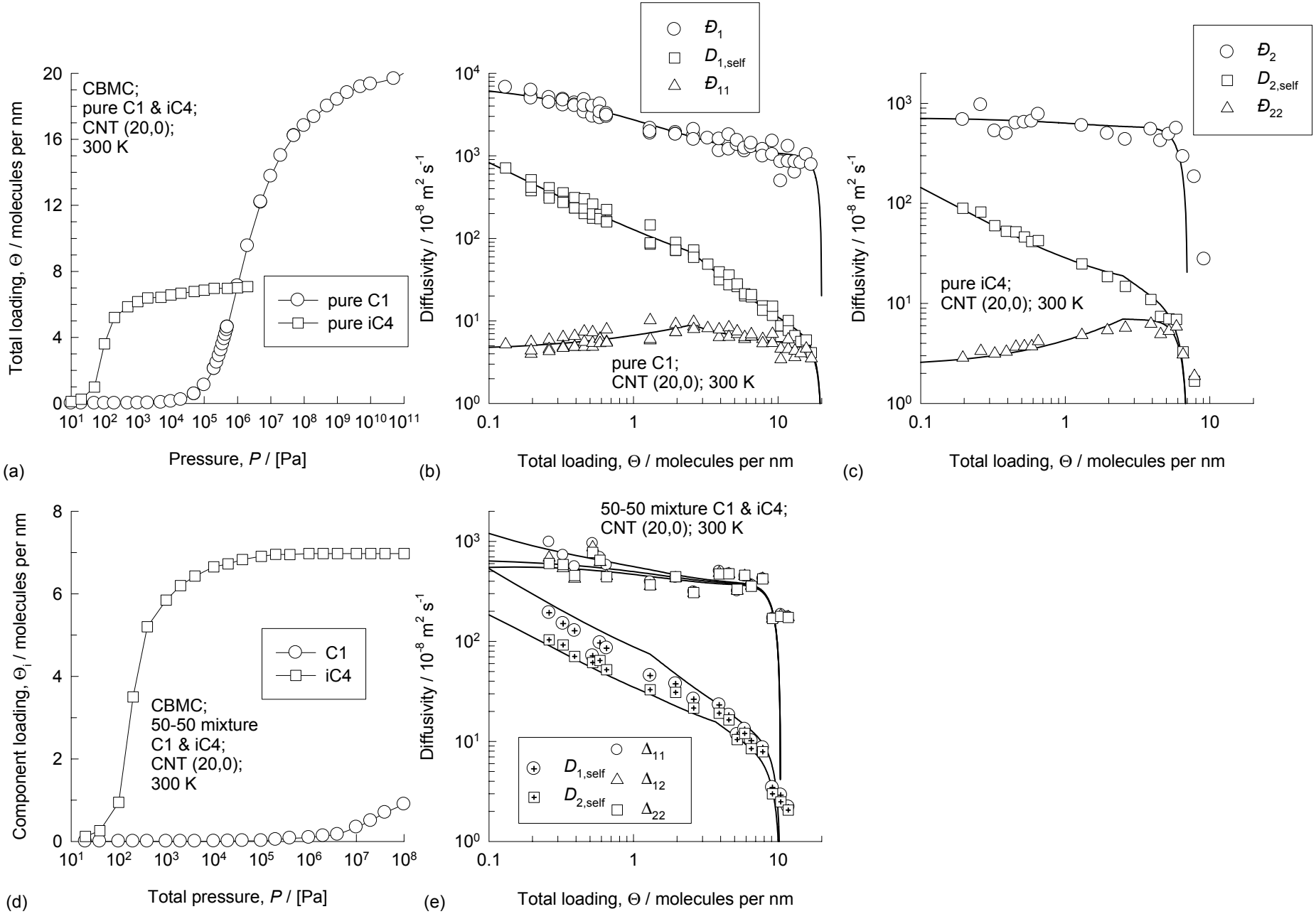
CNT (20,0); C1, nC4, and C1-nC4 mixture, 300 K



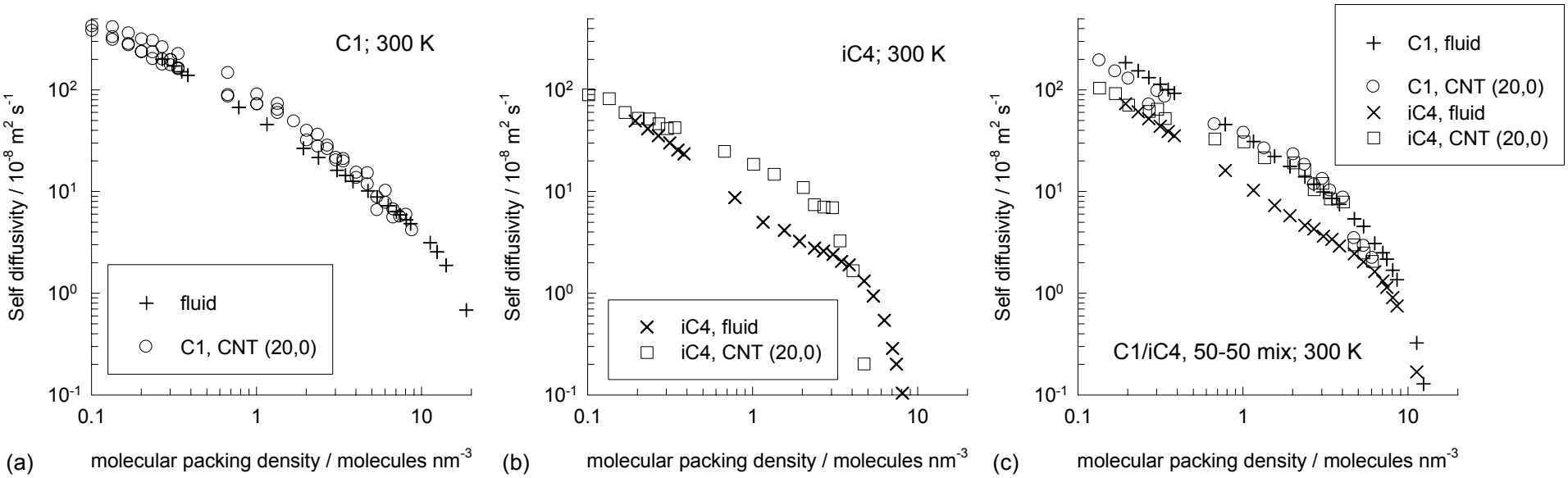
CNT (20,0) vs Fluid; C1, nC4, and C1-nC4 mixture, 300 K



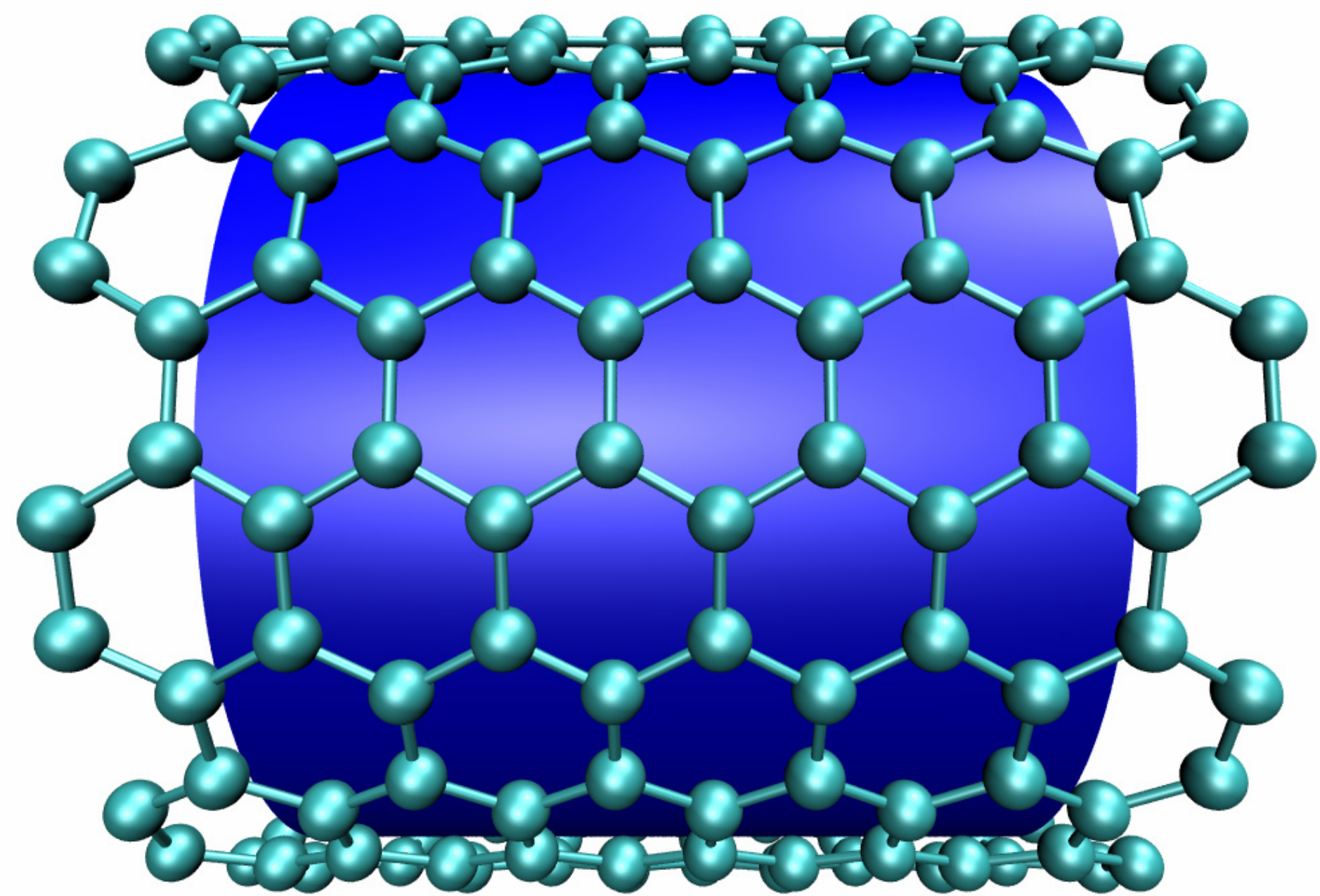
CNT (20,0); C1, iC4, and C1-iC4 mixture, 300 K



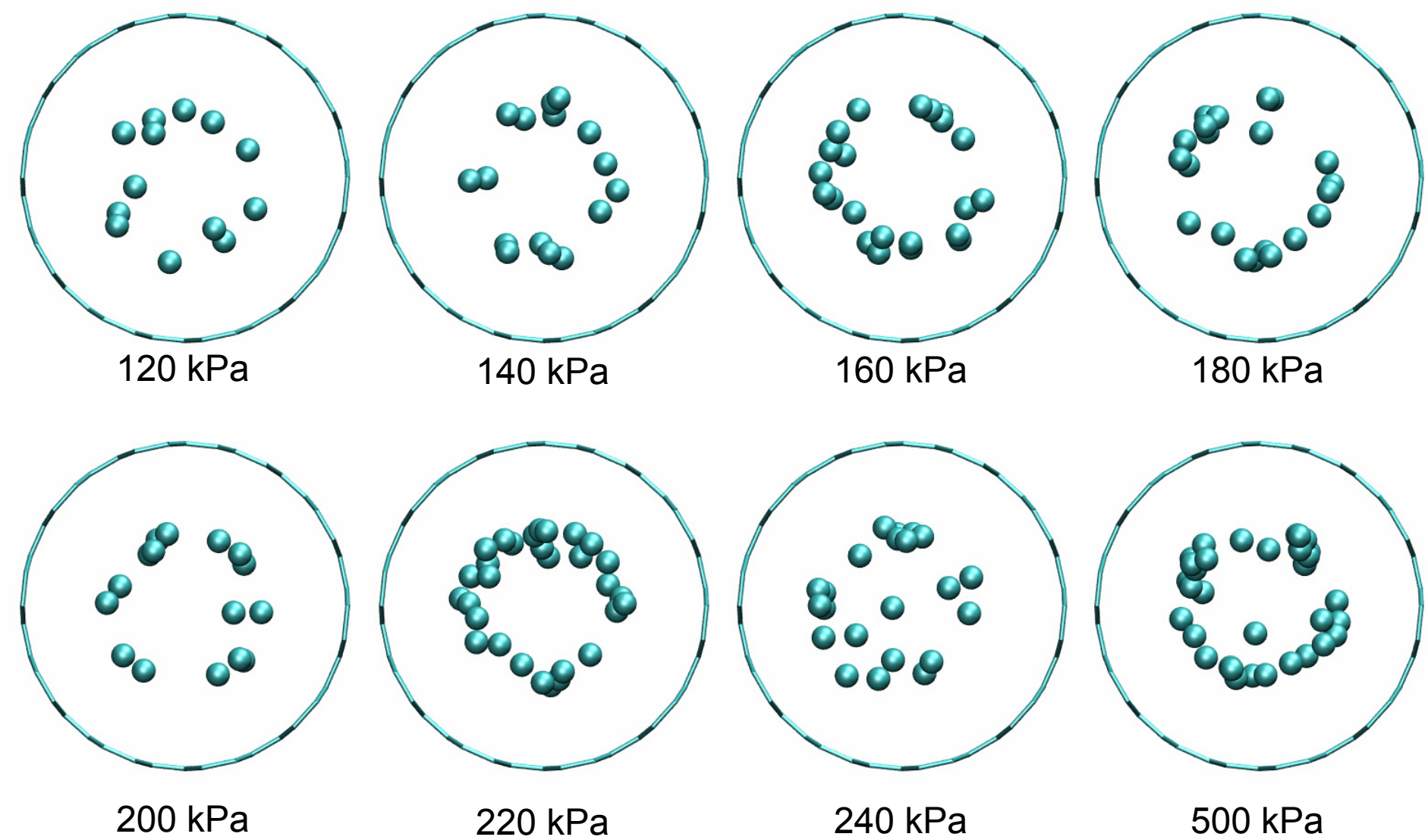
CNT (20,0) vs Fluid; C1, iC4, and C1-iC4 mixture, 300 K



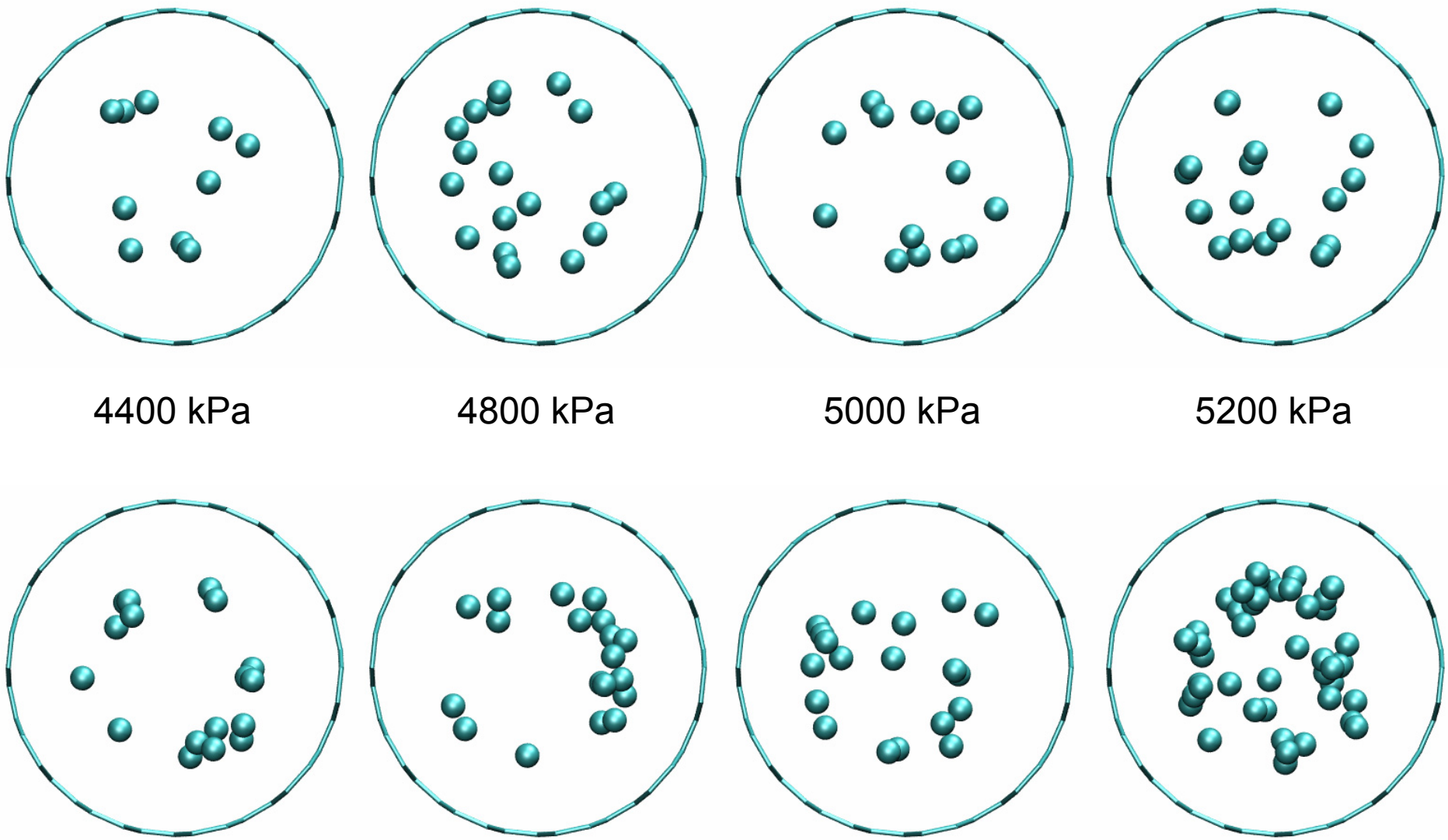
CNT (10,10)



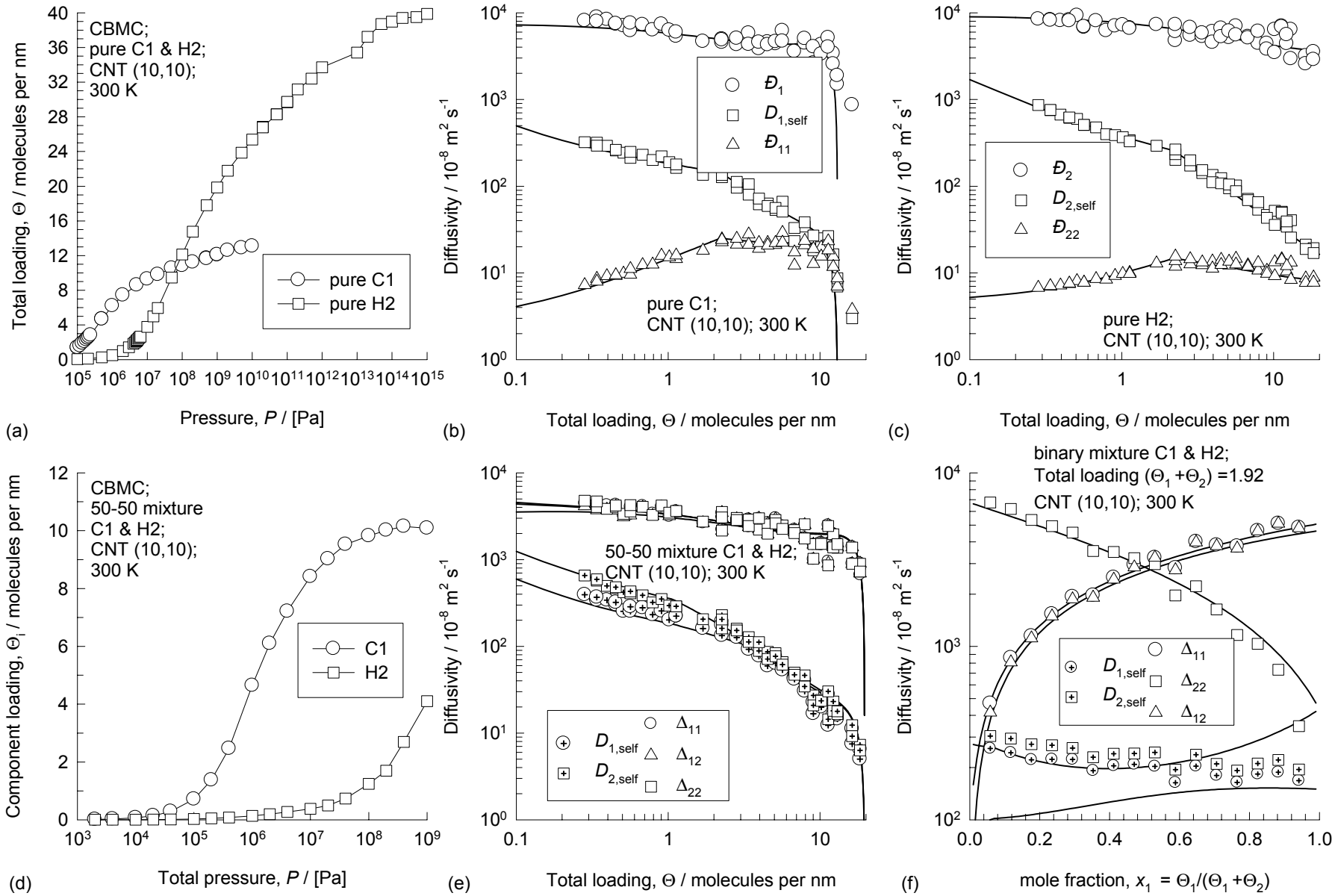
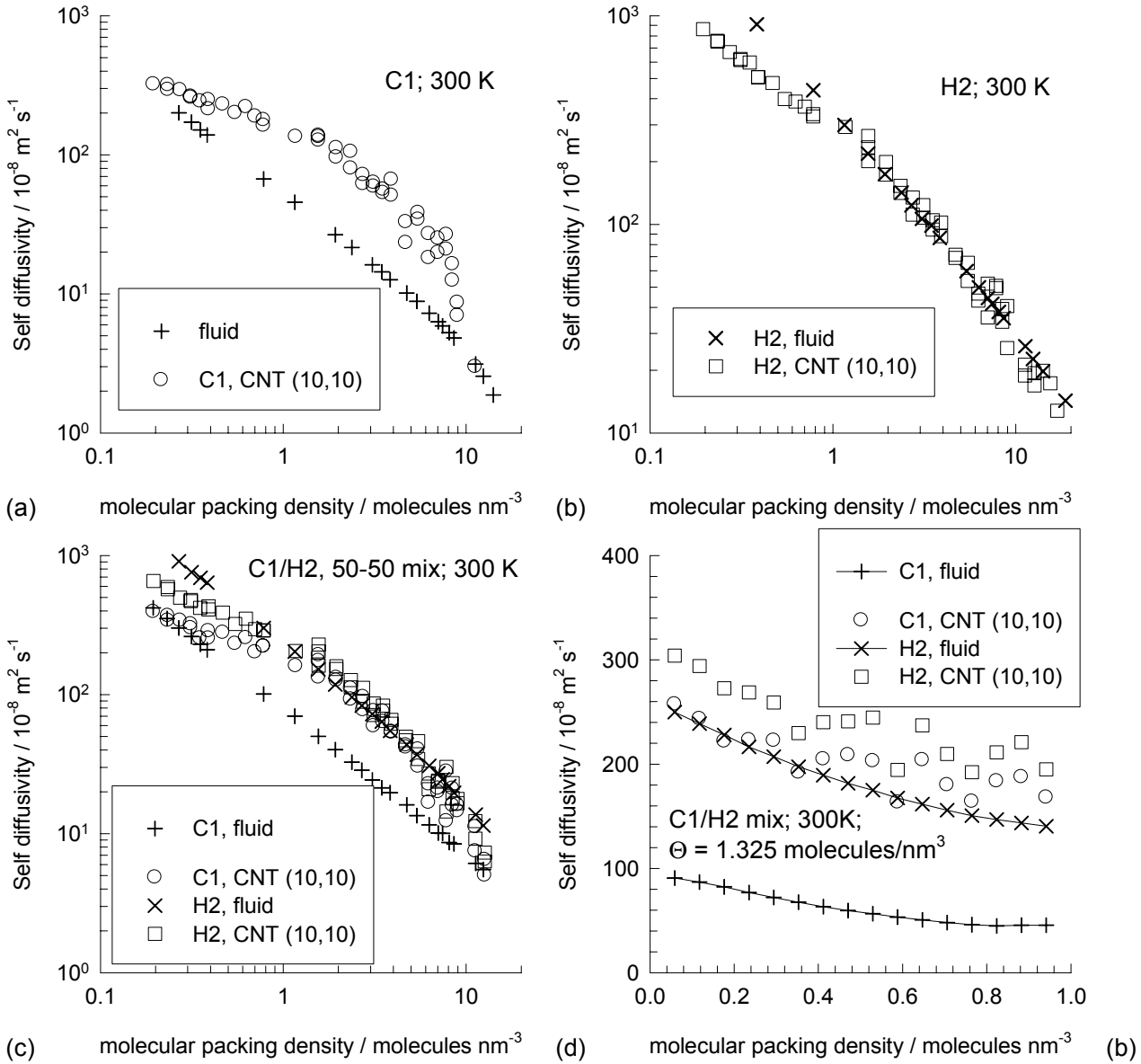
CNT (10,10); pure C1 adsorption, snapshots, 300 K



CNT (10,10); pure H2 adsorption, snapshots, 300 K



CNT (10,10); C1, H2, and C1-H2 mixture, 300 K



CNT (10,10) vs Fluid; C1, H2, and C1-H2 mixture, 300 K