Electronic Supplementary Material (ESI) for Molecular Systems Design & Engineering.

Role of Structural Rigidity and Collective Behaviour in the Molecular Design of Gas Hydrates Antiagglomerants

Supporting Information

François Sicard[1,2*] and Alberto Striolo[2]
[1] *Department of Physics and Astronomy, University College London, WC1E 6BT London, UK and*
[2] *Department of Chemical Engineering, University College London, WC1E 7JE London, UK*

*Corresponding author: francois.sicard@free.fr.

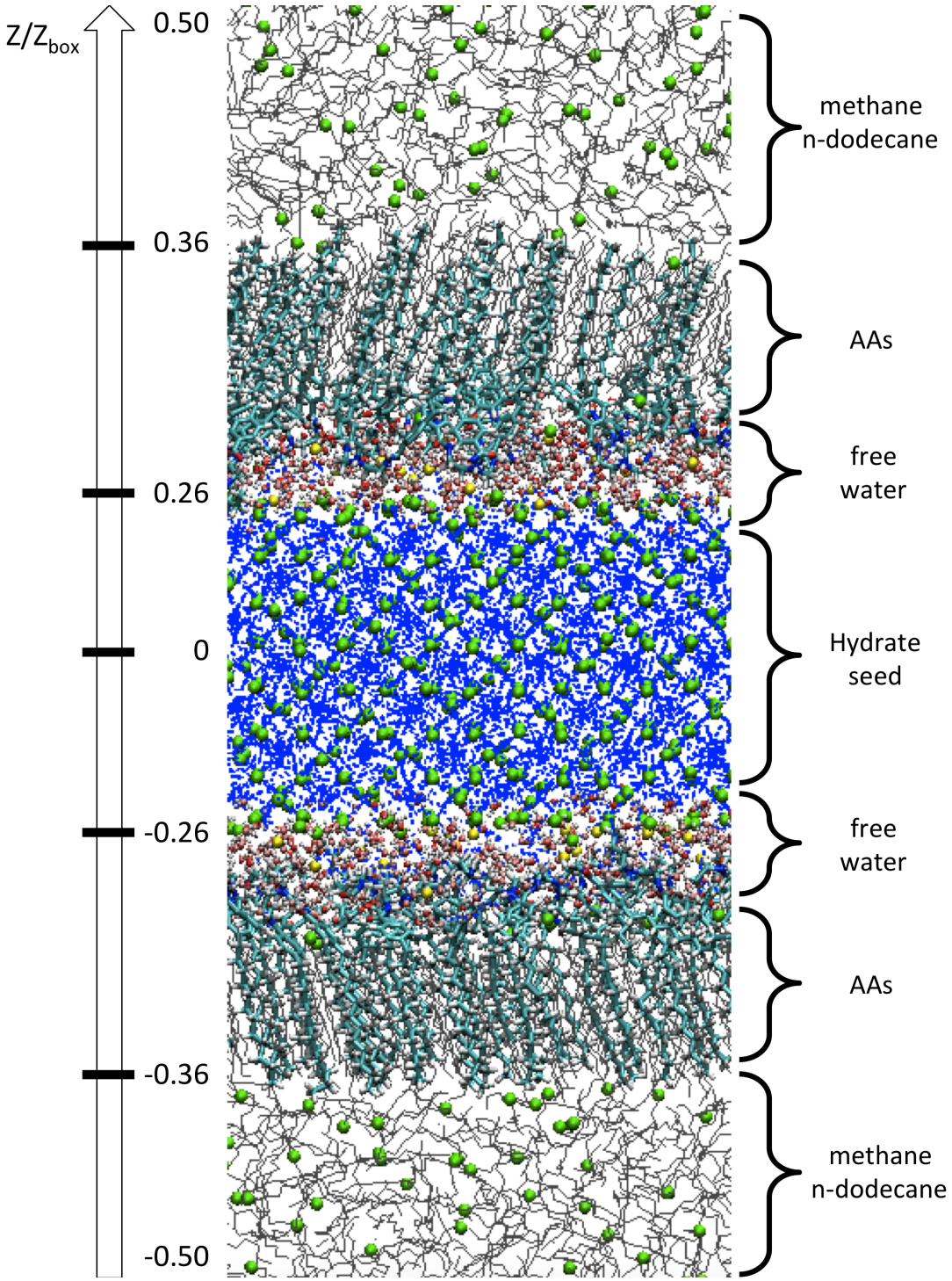

FIG. S1: Simulation snapshot of the whole system configuration obtained after equilibration with AAs with the aromatic ring positioned at the bottom of the hydrophobic tails and for an AA surface density ≈ 0.67 molecule/nm^2. Green spheres represent methane molecules either in the sII methane hydrate or the hydrocarbon phase. Blue dot lines represent water molecules in the hydrate substrate. Silver lines represent *n*-dodecane molecules, either in the bulk or trapped within the AA layer. Yellow, red, blue, white, and cyan spheres represent chloride ions, oxygen, nitrogen, hydrogen, and carbon atoms in AA molecules, respectively.

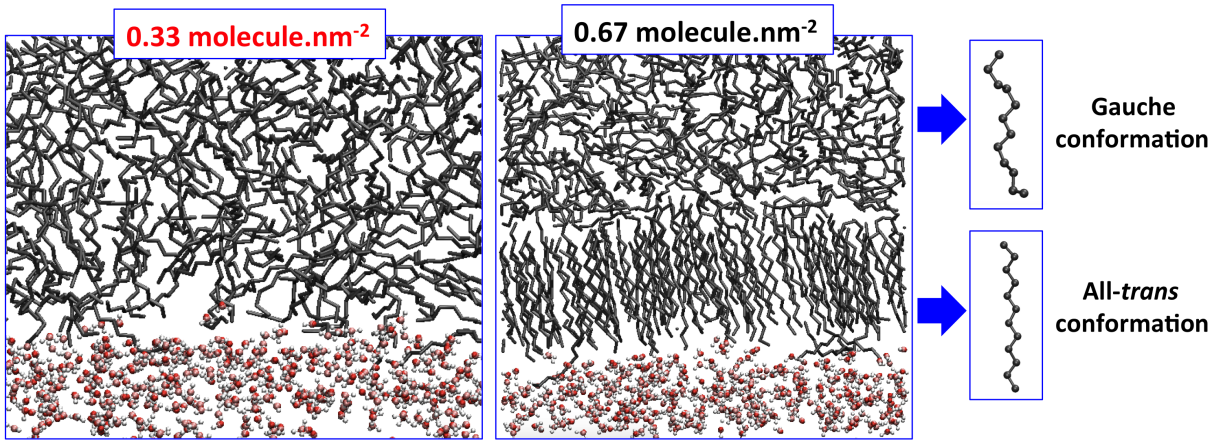

FIG. S2: Simulation snapshots for *n*-dodecane molecules within the AAs layer at different surface densities. The increase in AA surface density, which yields a transition between disordered to ordered orientation of the AA long tails (not shown here for clarity), comes with the configurational change of the *n*-dodecane molecules from a *Gauche* conformation in the bulk phase to a nearly *all-trans* conformation within the AA film.