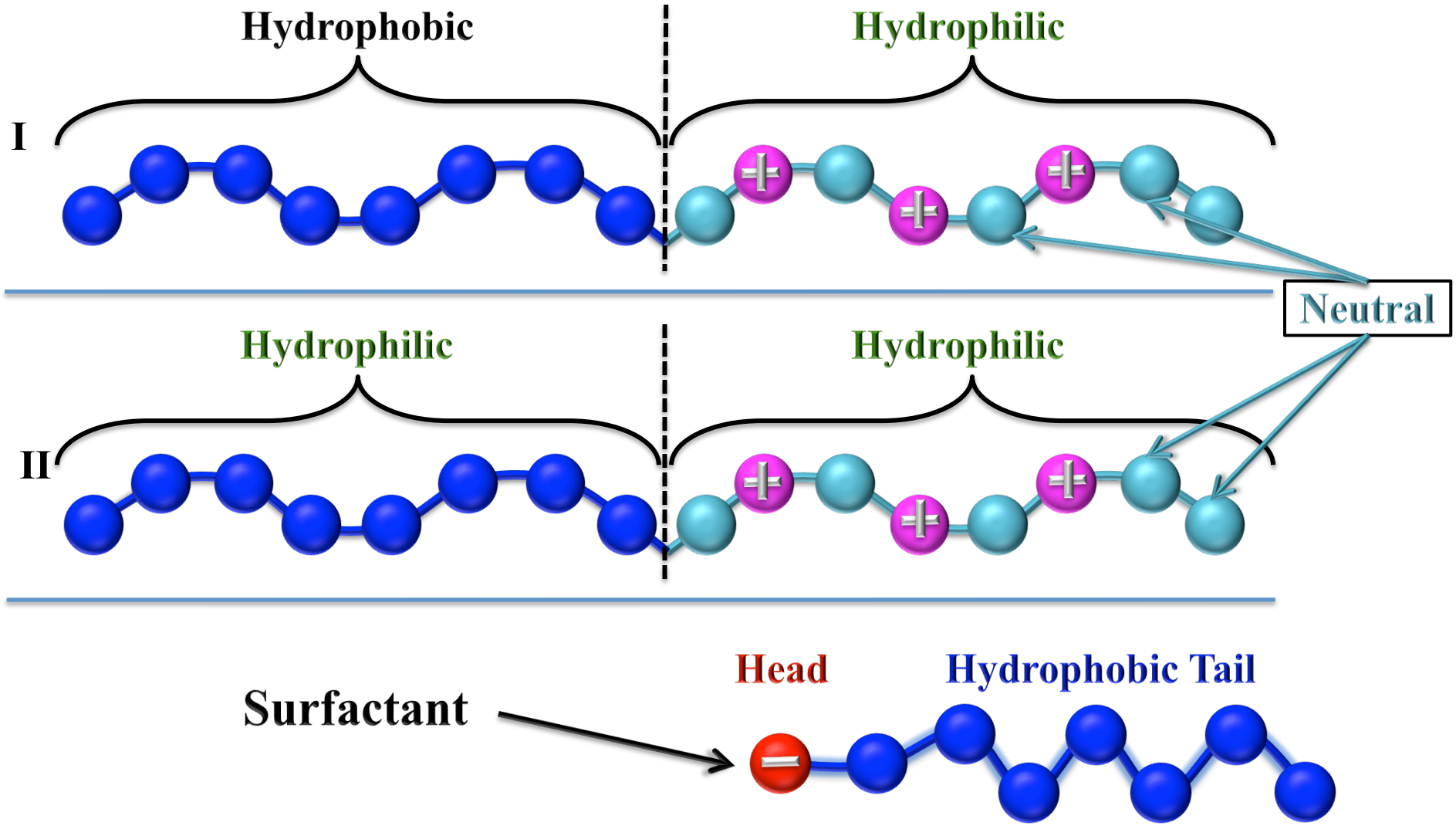
# Model Block-copolymers and Surfactants




Number of monomers on (50-50) block-copolymer chain: 60

Consists of 30 neutral sites, 30 cationic charged sites

Number of monomers on Surfactant: 12. 1 anionic head, 11 neutral tails.

**Each simulation was run for 10,000,000 LJ time steps. The trajectories are saved at 50,000 time step interval. So there are 20,000 trajectories in each file. The size of the monomer is sigma (monomer bead size).**

*System I: (Directory name :- Low_surf_conc): Trajectory file names description: (**Same as Figure System I**)*

# of polyelectrolyte (PE) chains: 400. PE chain length 60; 30 monomer charged block – 30 monomer neutral block. Each charged block contains 6 cations and 24 neutrals. # of surfactants: 1000; # of head 1000; # tail: 11*1000 = 11000:
So here are the breakup for different files:

1. "poly1.dat": all neutrals of the charged block, 24*400 = 9,600 molecules.
2. "poly2.dat": 30*400 = 12,000 molecules.
3. "polyCharge.dat": 6*400 = 2,400 molecules. Same in (Ncions.dat)
4. "head.dat": 1*1000 = 1,000 molecules (Same in "Pcions.dat")
5. "tail.dat": 11*1000 = 11,000

*System II: (Directory name :- Philic_BCP2): Trajectory file names description: (**Same as Figure System II**)*

# of polyelectrolyte (PE) chains: 100. PE chain length 60; 30 monomer charged block – 30 monomer neutral block. Each charged block contains 6 cations and 24 neutrals. # of surfactants: 1000; # of head 1000; # tail: 11*1000 = 11000:
So here are the breakup for different files:

1. "poly1.dat": all neutrals of the charged block, 24*100 = 2,400 molecules.
2. "poly2.dat": 30*100 = 3,000 molecules.
3. "polyCharge.dat": 6*100 = 600 molecules. Same in (Ncions.dat)
4. "head.dat": 1*1000 = 1,000 molecules (Same in "Pcions.dat")
5. "tail.dat": 11*1000 = 11,000

*System III: (Directory name :- Phobic_BCP2): Trajectory file names description: (**Same as Figure System I**)*

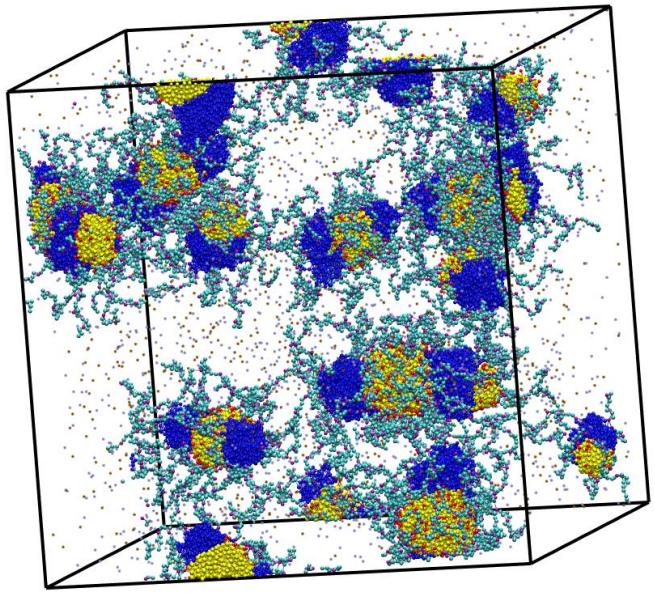
# of polyelectrolyte (PE) chains: 100. PE chain length 60; 30 monomer charged block – 30 monomer neutral block. Each charged block contains 6 cations and 24 neutrals. # of surfactants: 1000; # of head 1000; # tail: 11*1000 = 11000:
So here are the breakup for different files:

1. "poly1.dat": all neutrals of the charged block, 24*100 = 2,400 molecules.
2. "poly2.dat": 30*100 = 3,000 molecules.
3. "polyCharge.dat": 6*100 = 600 molecules. Same in (Ncions.dat)
4. "head.dat": 1*1000 = 1,000 molecules (Same in "Pcions.dat")
5. "tail.dat": 11*1000 = 11,000

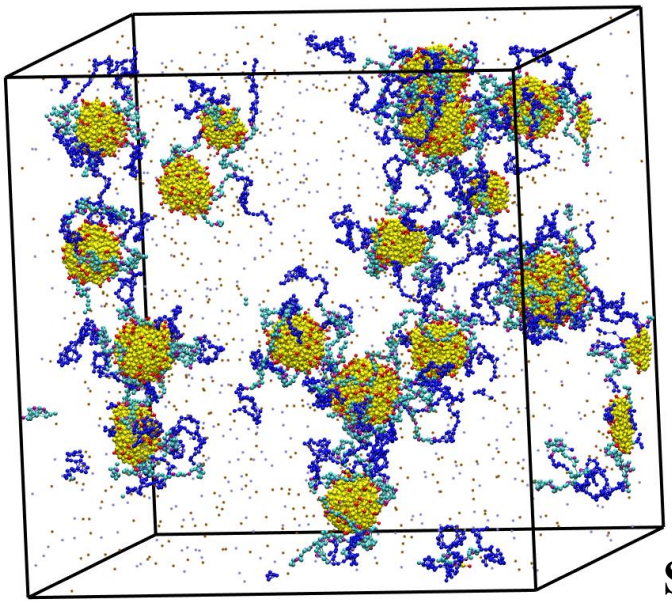
*System IV: (Directory name :- Strong_Phobic_BCP2): (**Same as Figure System I**)*

This system is same as System III above. All the molecule numbers and definition are the same as III. The only difference is the hydrophobic interactions with the PE hydrophobic part and Surfactant tail is 2 times stronger.

I. Low_surf_conc



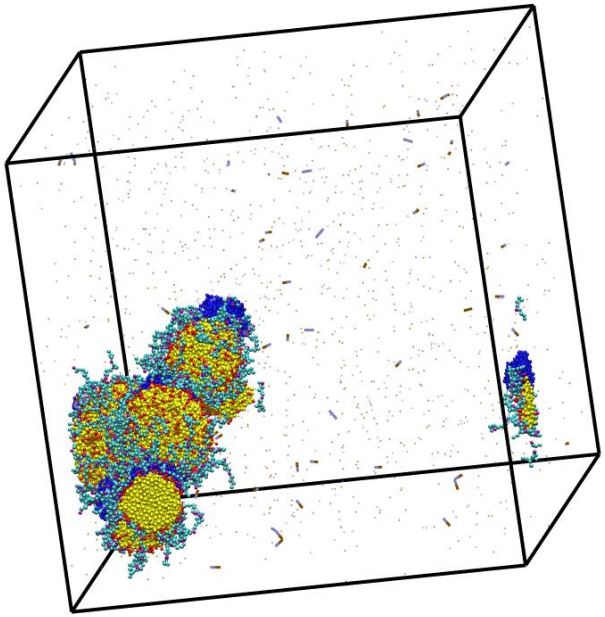
II. Philic_BCP2



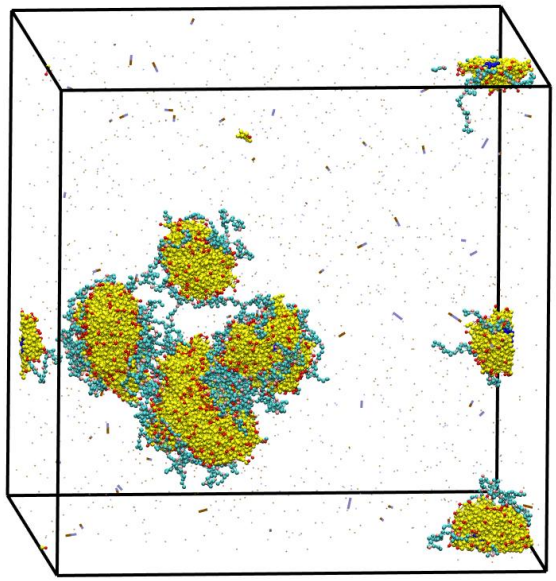
Blue: PE neutral
Cyan: PE charge block
Purple: PE charge
Yellow: Surfactant tail
Red: Surfactant head

Small dots inside the boxes are counterions.

III. Phobic_BCP2



IV. Strong_Phobic_BCP2



Same Figure IV but with PE neutral shown inside surfactant cluster