Institute of Fundamental Technological Research
Polish Academy of Sciences

POWSTAWANIE NANOSTRUKTUR W EMULSJACH

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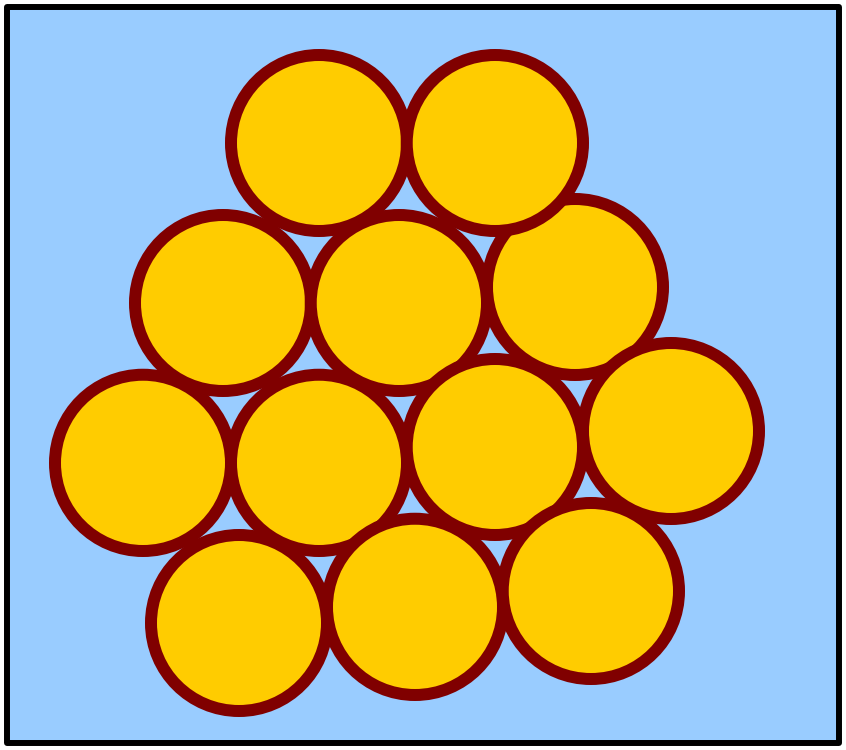
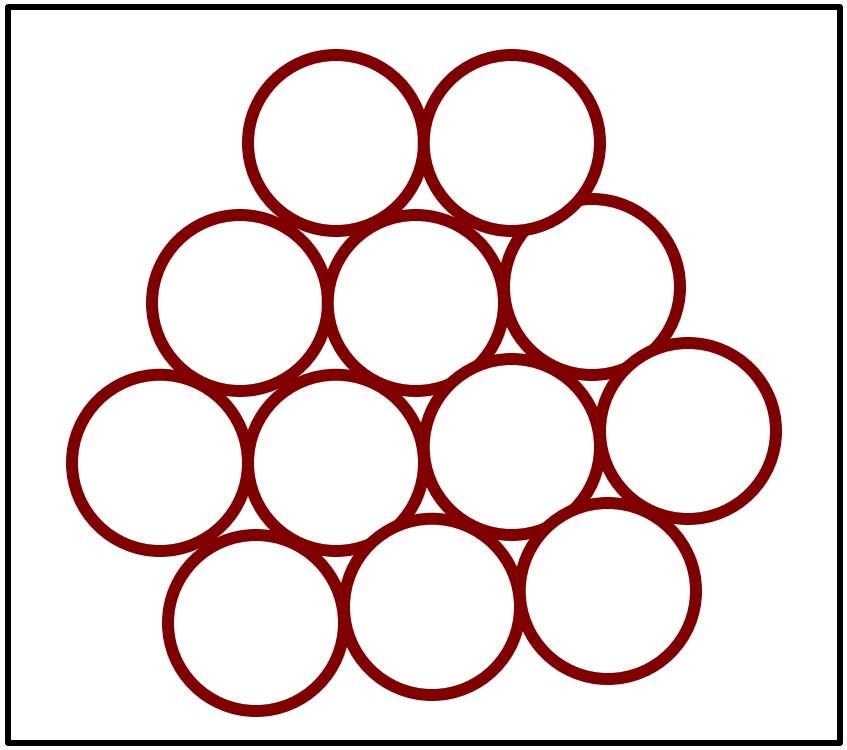
Aim of CONEX project - Nanomaterials



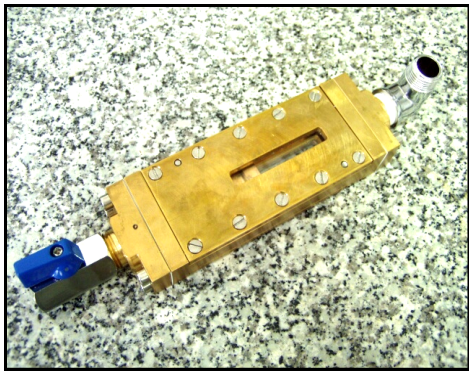
The emulsion with thin layers of third substance at the surface between oil and water

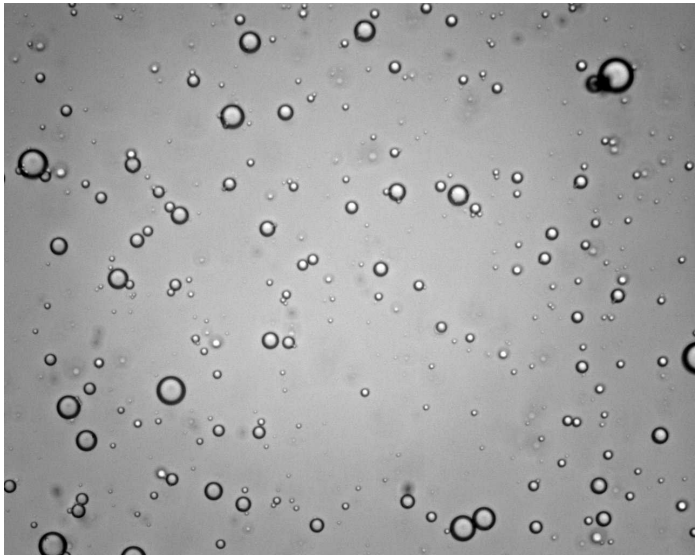


The structure of nanomaterial after removing water and oil

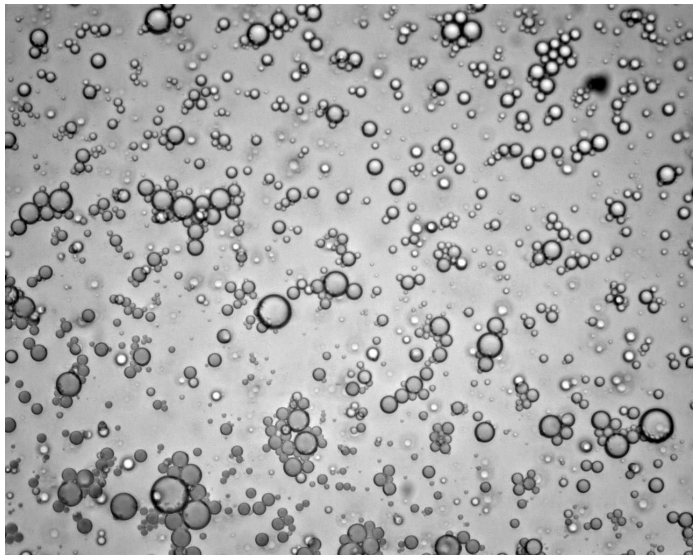
Experiments

The picture of homogenizer used in laboratory experiments





d~10μm

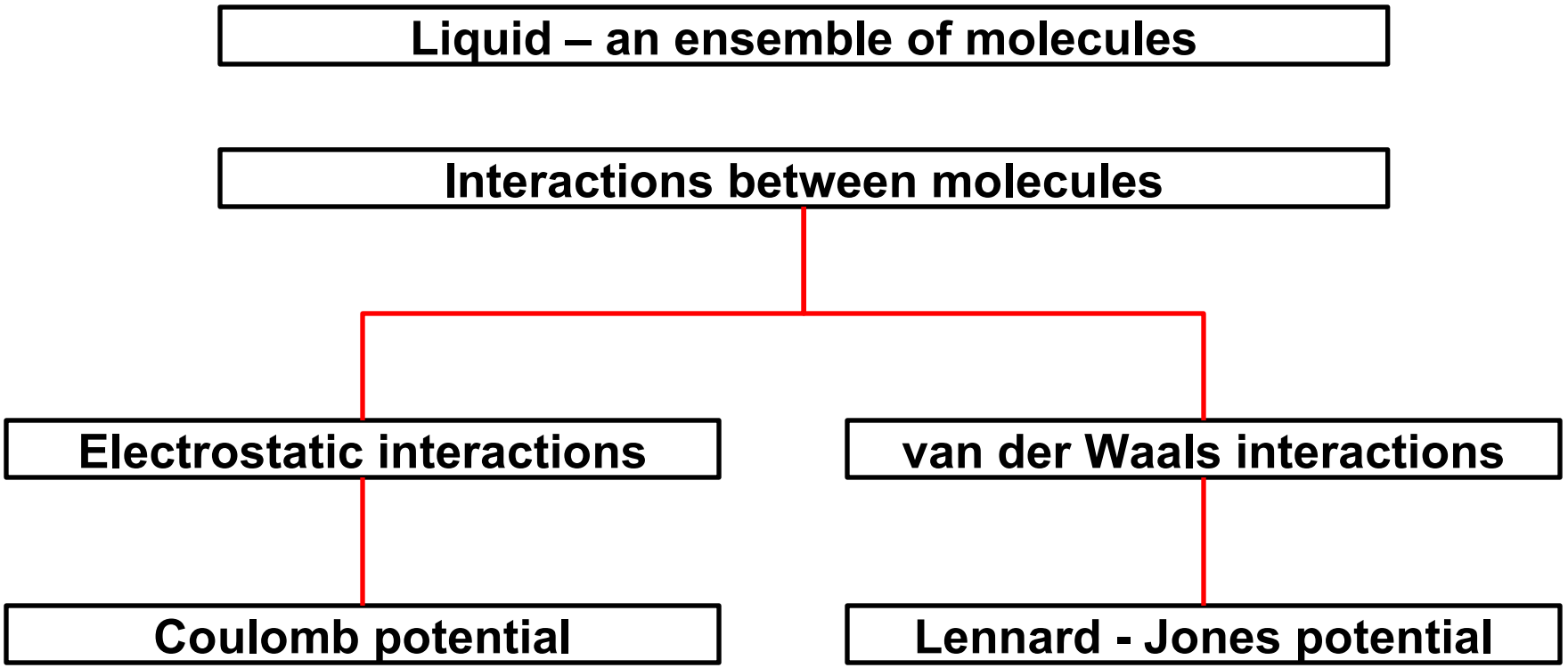


d~20μm

The pictures of the emulsions maked by the homogenizer.

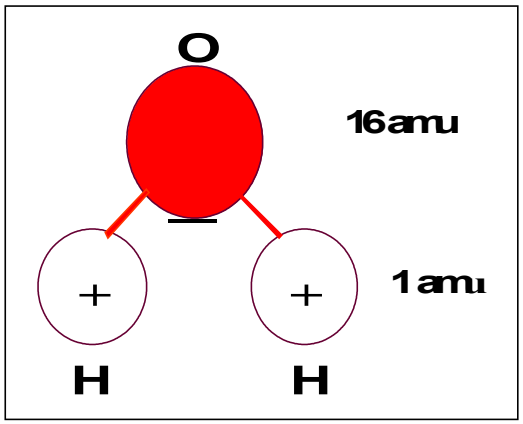
Sławek Błoński ZMiFP

Molecular Dynamics Simulation



The program „Moldy” by Keith Refson used for simulation.

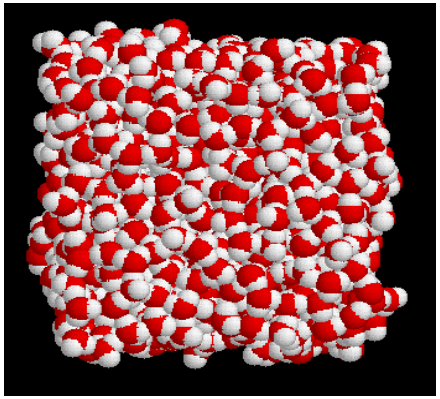
Formation of water droplet in vacuum



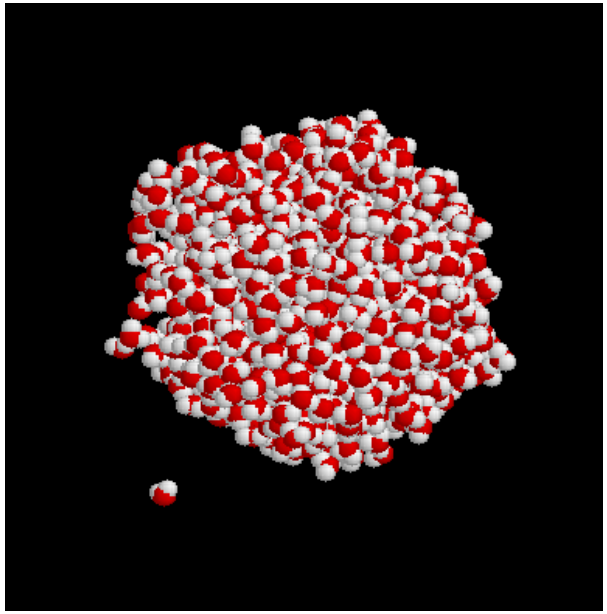
Molecule of water

Molecules of water = 1000

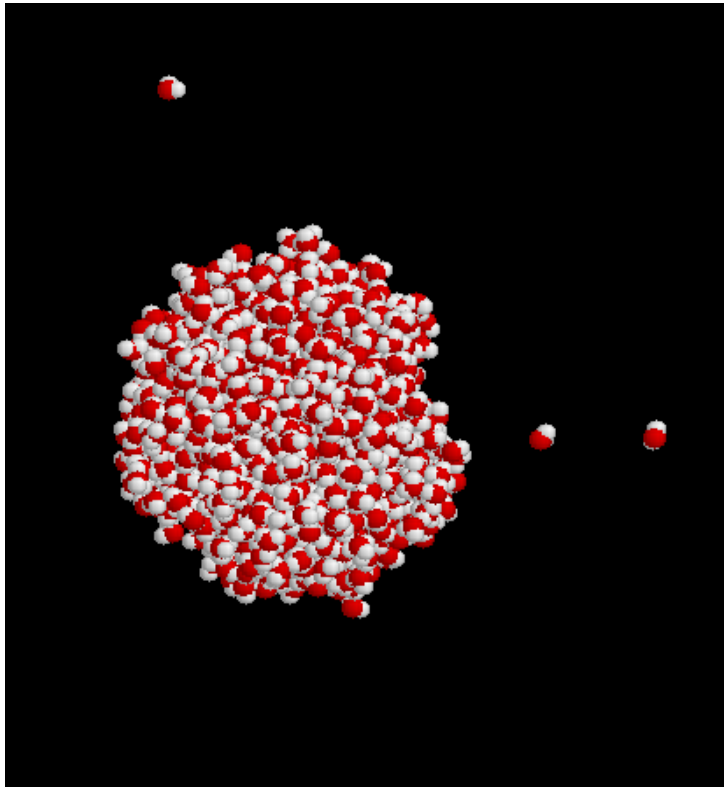
Diameter of the droplet ~38 Å



t = 0 ps



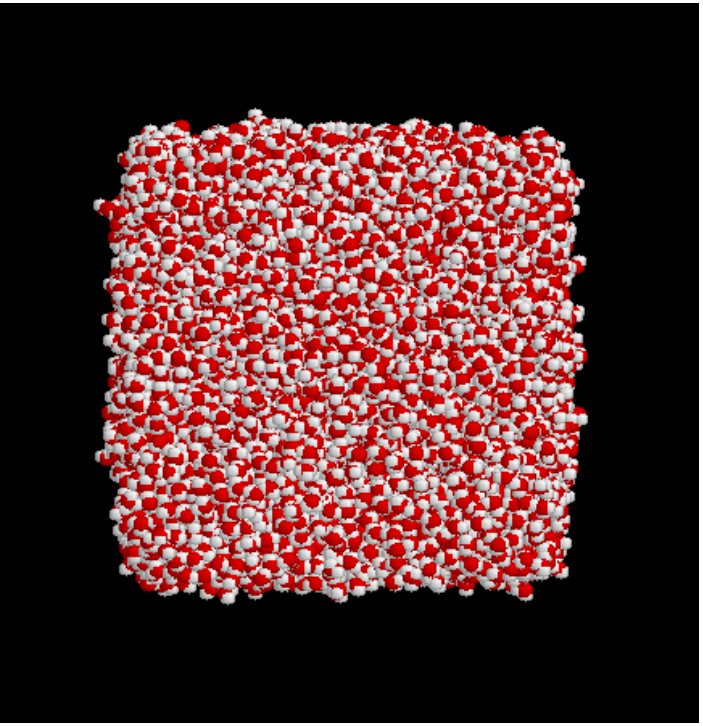
t = 8 ps



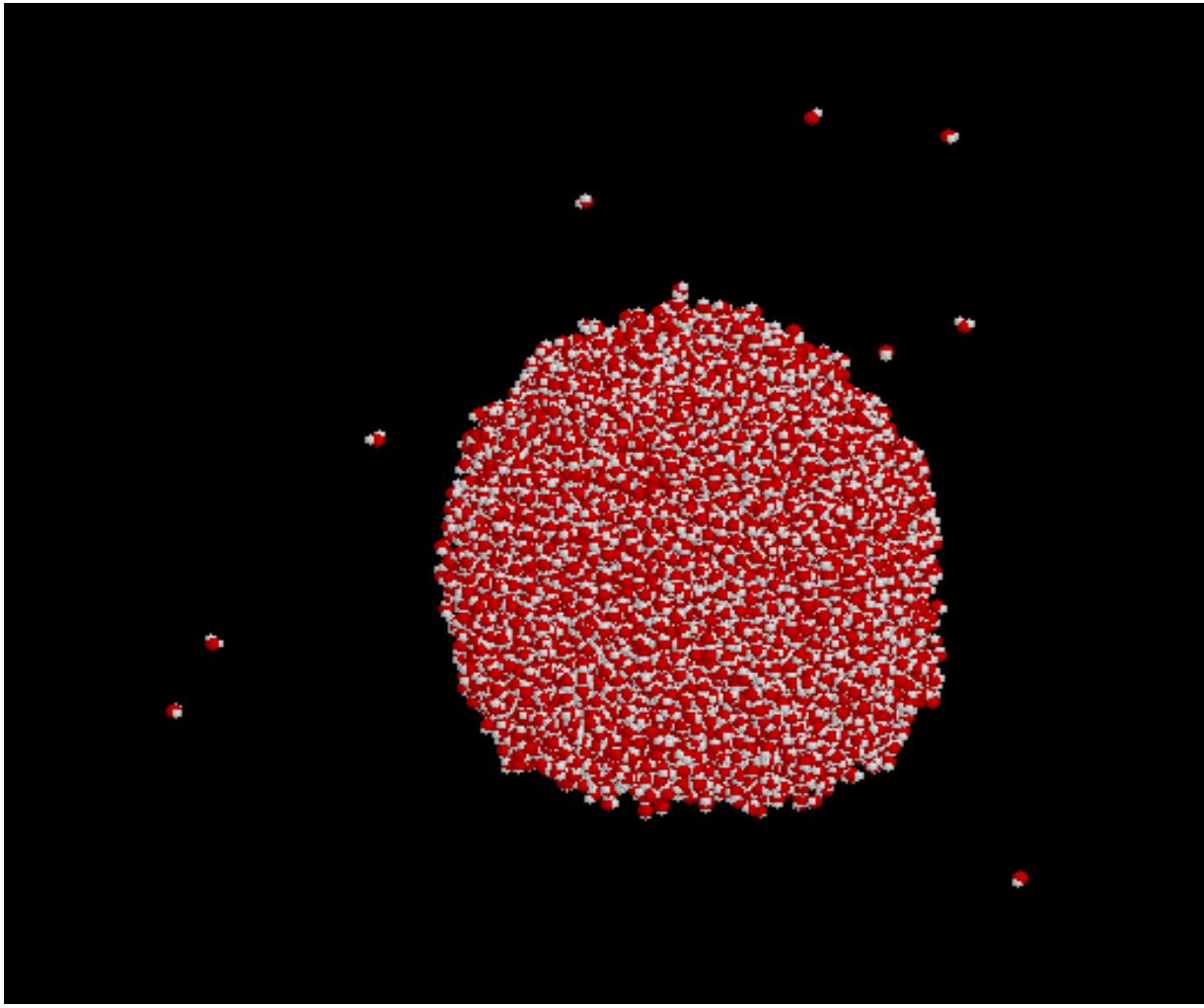
t = 40 ps

Molecules of water = 10648

Diameter of the droplet ~84 Å



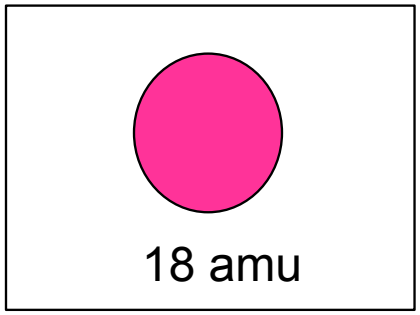
t = 0 ps

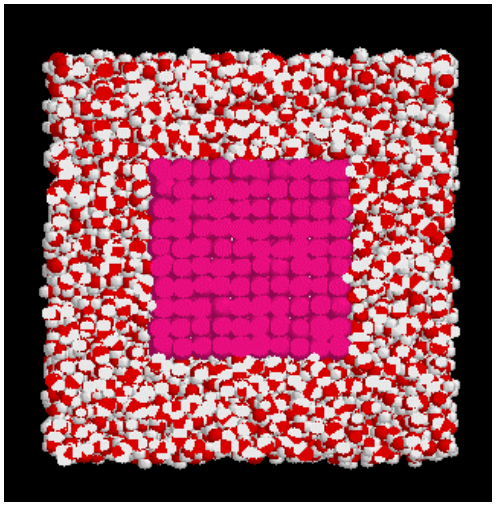


t = 16 ps

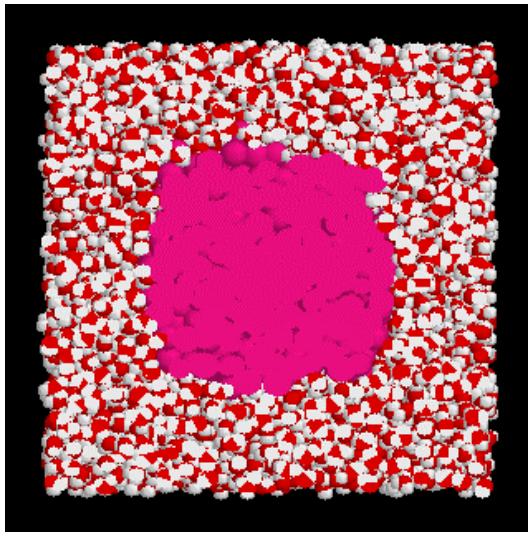
Simulation of emulsification process

Model of oil

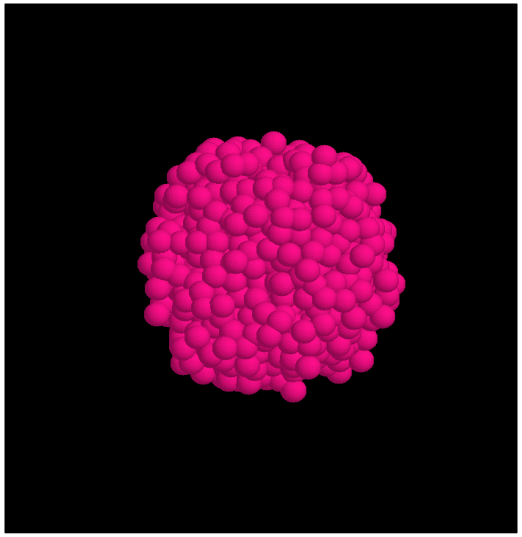




t = 0 ps

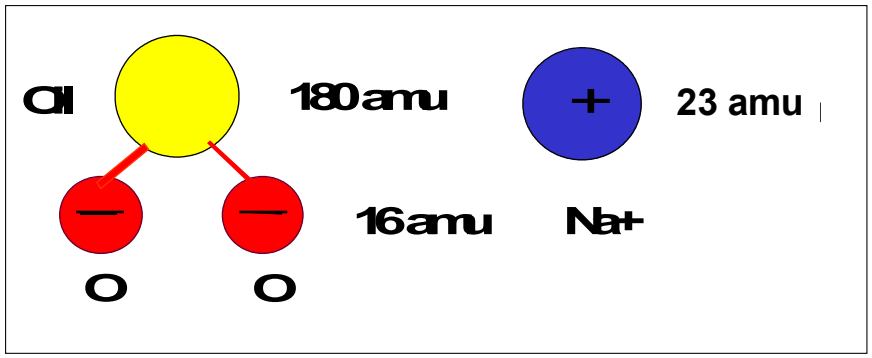


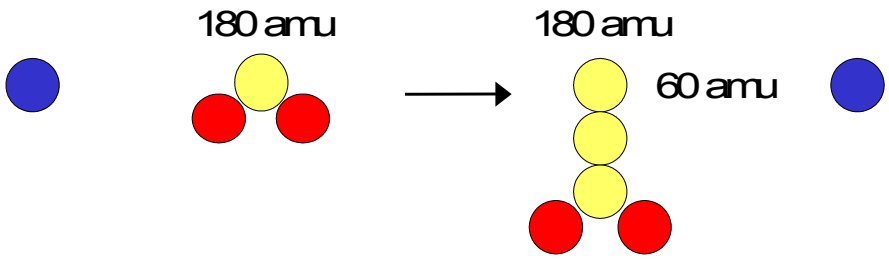
t = 5ps

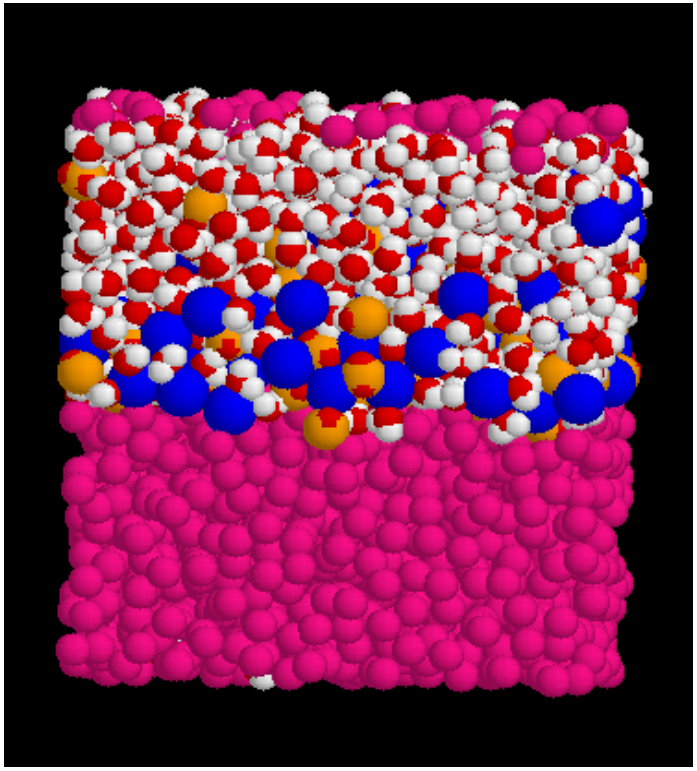


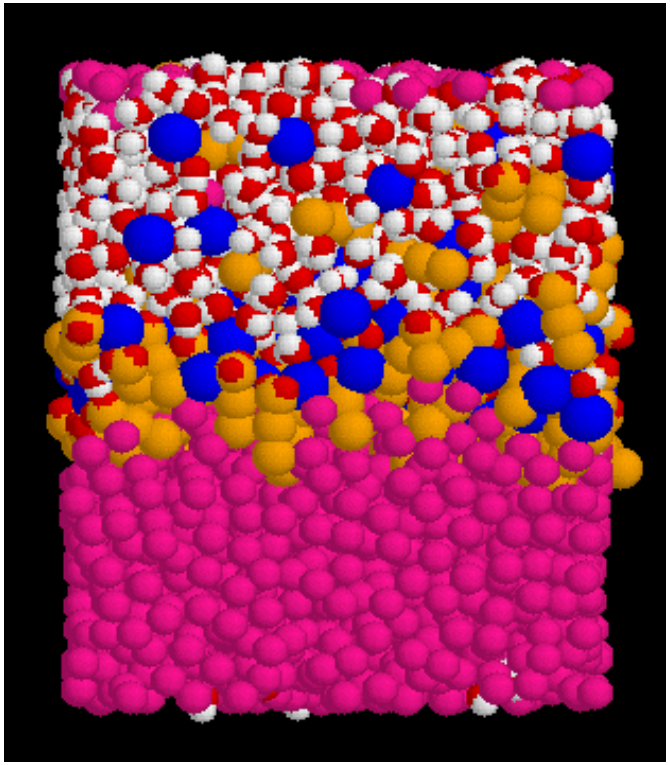
t = 13ps

Simulations of three liquids:”short” and ”long” soap



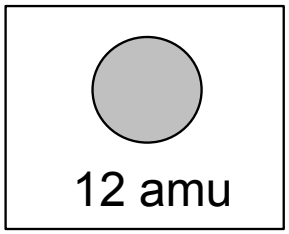




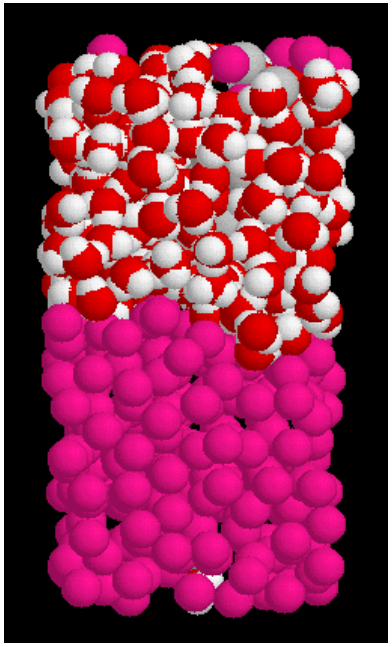


Simulations of two liquids and solid

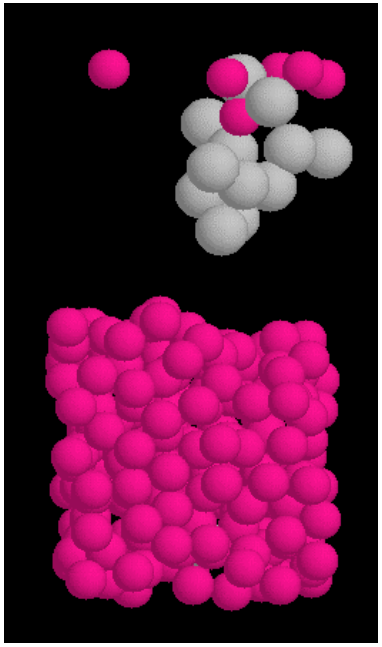
Model of carbon

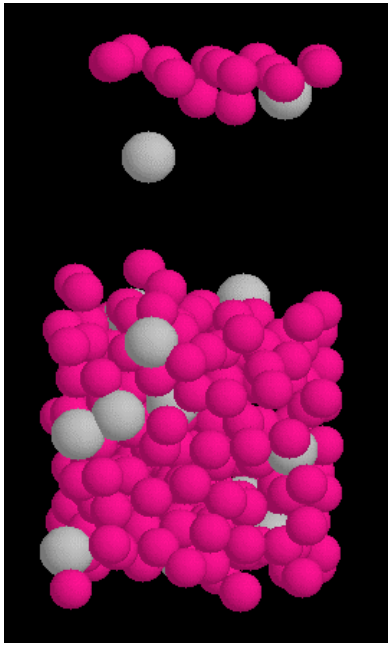


Atomic form of carbon

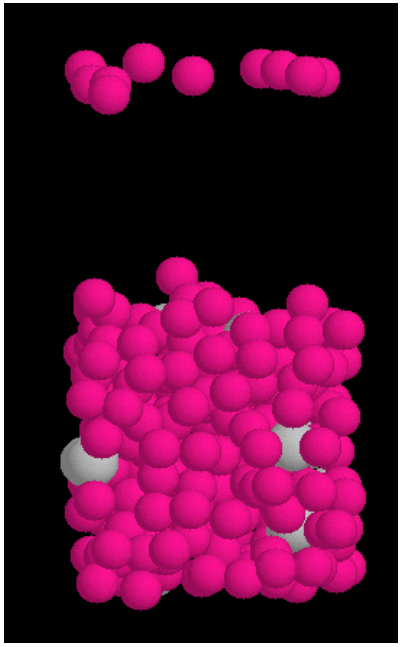


t = 0 ps



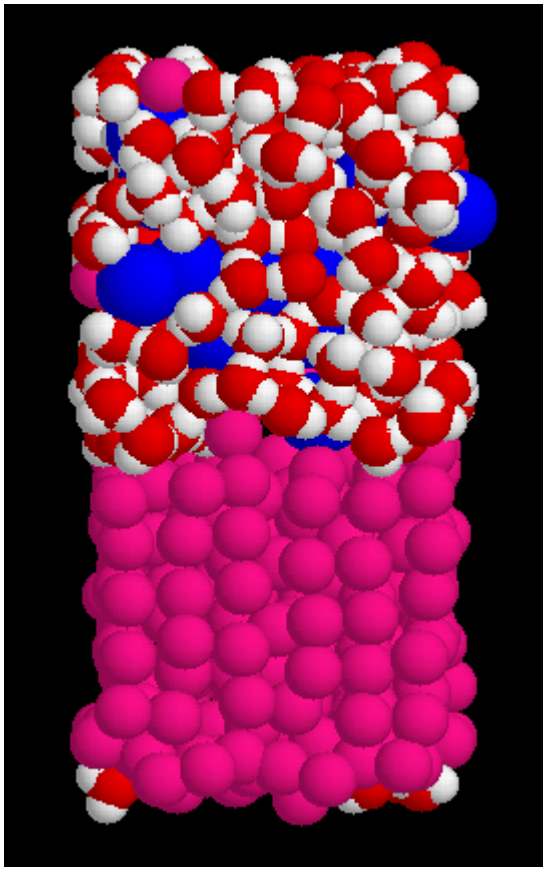


t = 115 ps

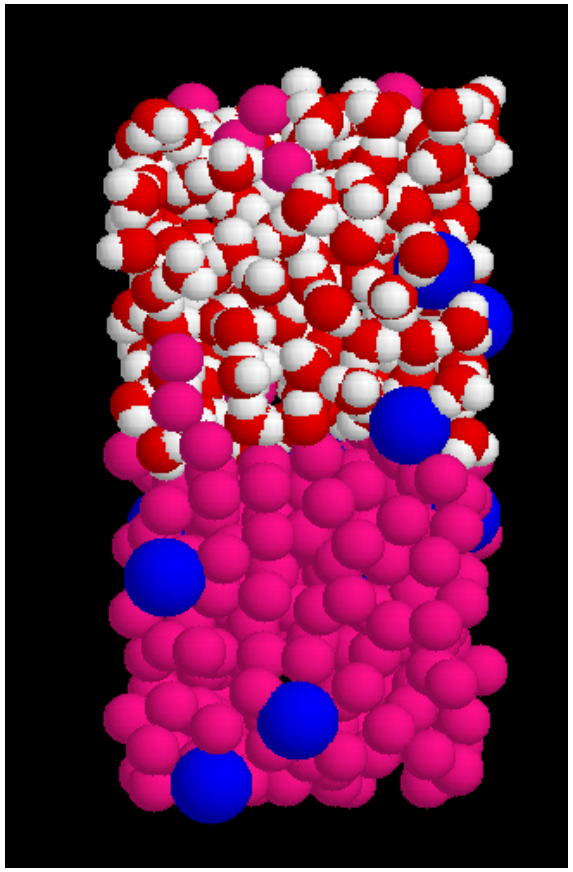


t = 165 ps

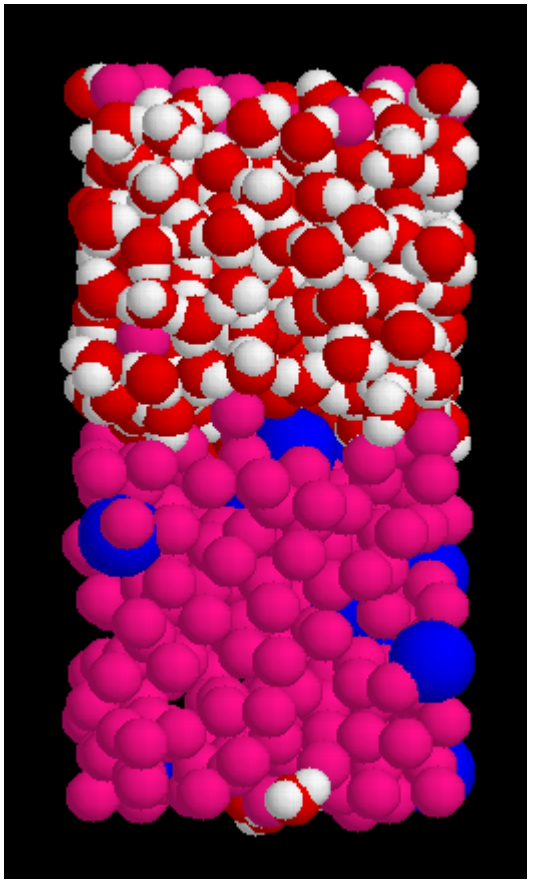
Quasi-Carbon



t = 0 ps



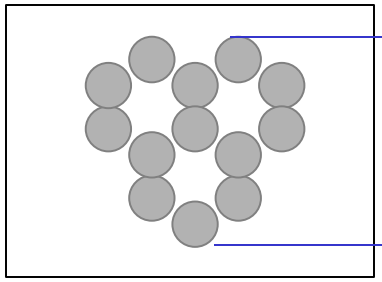
t = 100 ps



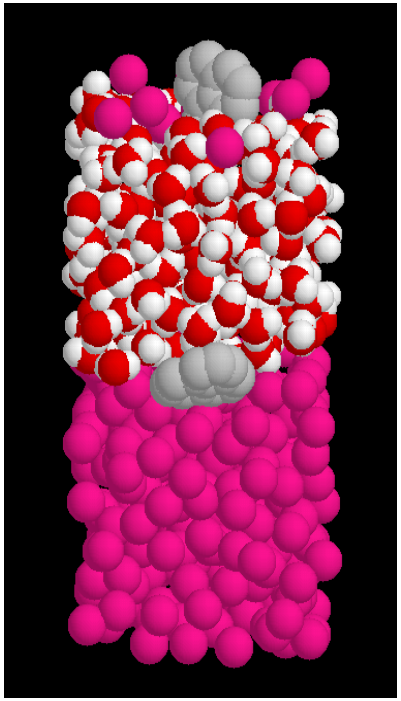
t = 500 ps

Simulations of emultion and complex of carbon

Model of carbon complex

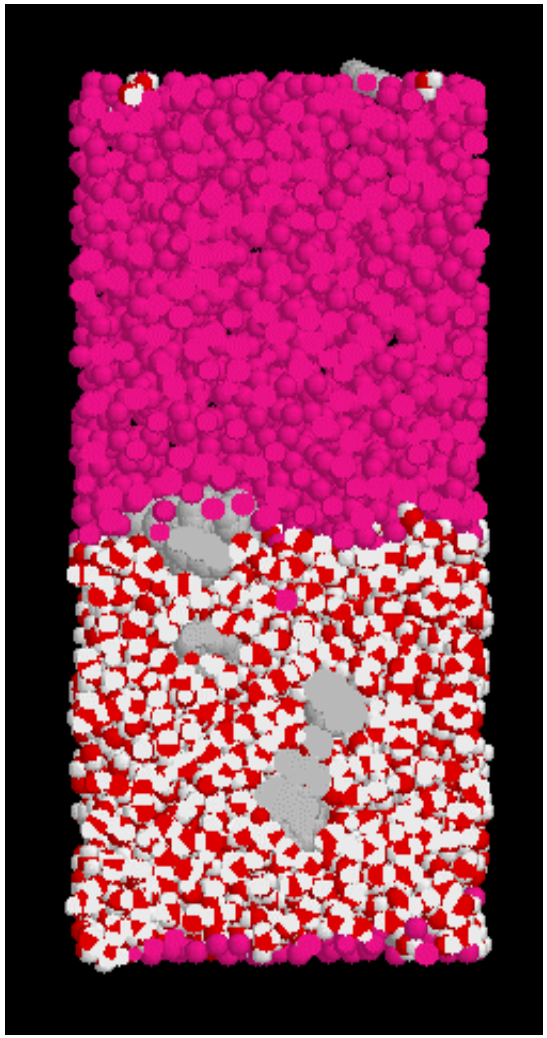


~ 0.8 nm



t = 206 ps

~ 4,6 nm

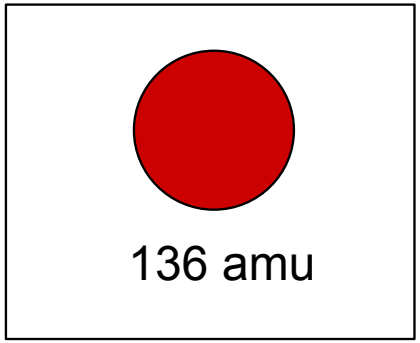


t = 132 ps

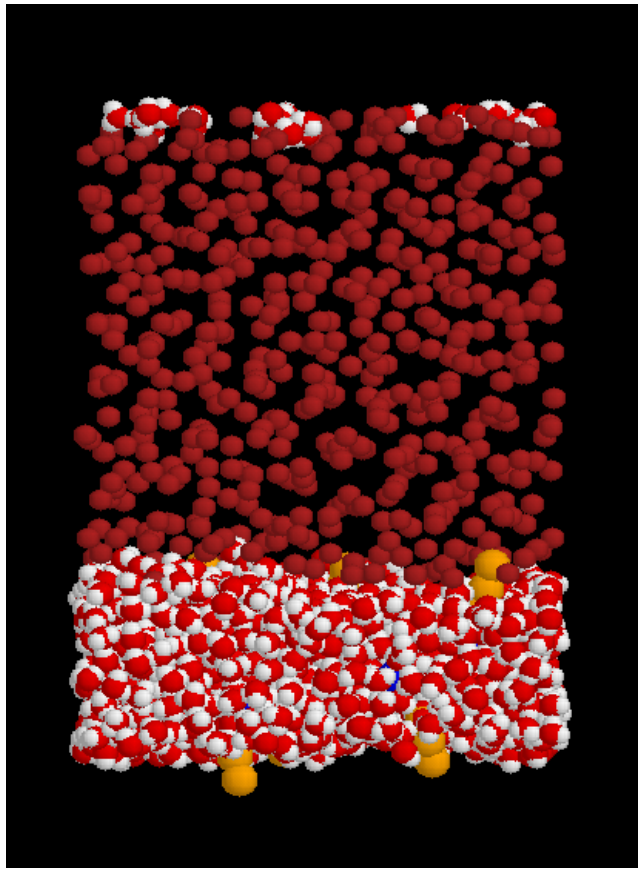
Simulations of water and limonene emulsion...

Limonene:
aromatic, voletail oil

Model of limonene

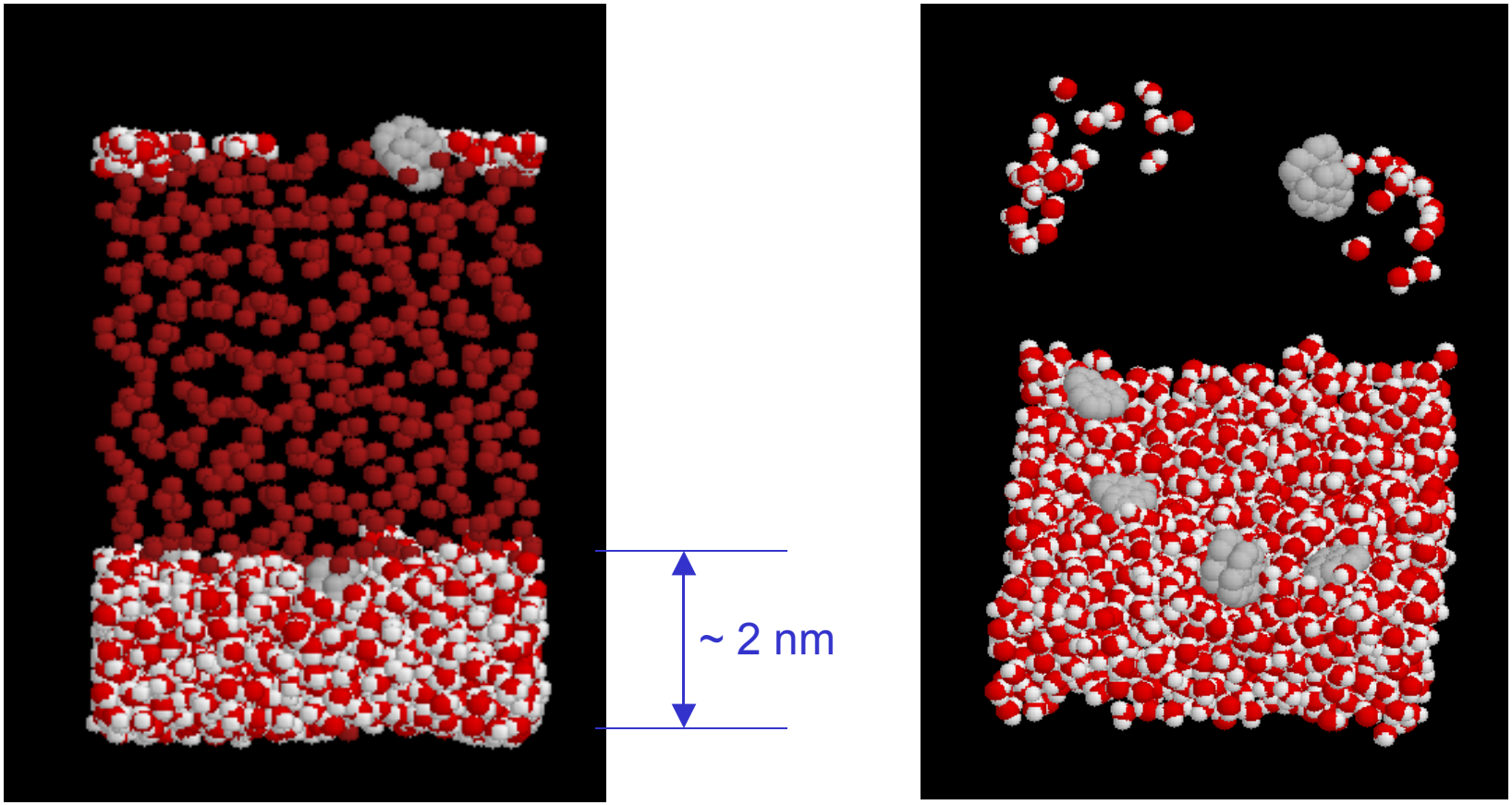


...with soap



t = 300 ps

...with carbon complexes



t = 100 ps

Conclusions

• Metoda dynamiki Molekularnej jest dobrym narzędziem do opisu zjawisk zachodzących w cieczach na poziomie nanometrów.

• Do opisu efektu rozdzielenia cieczy w emulsji złożonej z oleju i wody przyjęto modele molekularne uwzględniające hydrofilowe i hydrofobowe oddziaływania między cieczami.

• Wydłużenie łańcucha olejowego w cząsteczce surfaktantu stabilizuje proces tworzenia się jego warstwy na granicy faz emulsji.

• Węgiel w postaci atomowej przechodzi z fazy wodnej do olejowej.

• Kompleksy węgla osiadają na powierzchni styku faz emulsji. Proces osadzania przyspiesza użycie cienkiej warstwy wody.