Molecular Dynamic Simulations of Hydrocarbon Mixtures and Ionic Liquids with GROMACS

The aim of this course is to introduce some basic concepts around molecular dynamic simulations by means of making an example, in this case, the mixture of Hydrocarbons and Ionic Liquids. One possible application of this strategy is to reduce the concentration of benzene in gasolines by means of ionic liquids.

Day 1

1. Introduction to Molecular Dynamics simulations.
2. Aromatic compounds dangers to human health and environment.
3. Ionic Liquids as an alternative solvent.
4. Making a model of gasoline and a model of ionic liquid.

Day 2

1. Some results about extraction of benzene from gasoline by means of Ionic Liquids.
2. Making a mixture of gasoline and ionic liquid.

Previous Software requirements

- Linux or MacOS
- Gnu (gfrotran, gcc, etc.) or Intel compilers
- GROMACS 5.1.2 http://manual.gromacs.org/documentation/
- VMD http://www.ks.uiuc.edu/Research/vmd/
- Grace http://plasma-gate.weizmann.ac.il/Grace/

Other requirements

- Basic knowledge of shell commands

Instructor

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