Title: **Molecular dynamics simulations of liquid-liquid and liquid-gas interfacial tensions for several systems with water and organic compounds.**
Student: Yago Mena Barrientos
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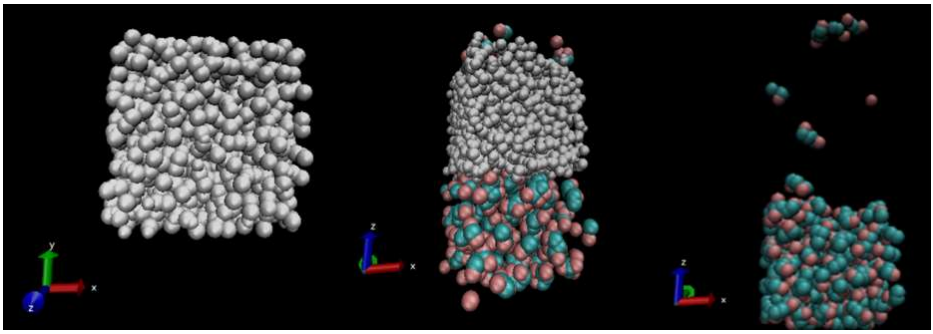
Supervisor/s: Dr. Ramón Sayós Ortega
Departament de Ciència de Materials i Química Física

1. SUMMARY

Nowadays, one of the most effective, fast and cheap methods to predict the physicochemical properties of matter, on a certain system, is by using molecular dynamic simulations (MD), this method was first developed in the late 50s in the field of theorical physics, and has been improving until recent days, currently is mostly used in the fields of chemical physics, material science and in the research and development of biomolecules for pharmaceutical industry.

Complex systems with a large number of molecules experience experimental problems to determine their physicochemical behaviour. Molecular dynamic simulations present less errors, however it is not a completely error free method, the errors accumulated by the integration of the speed equations end up giving deviations in the results to a greater or lesser extent, according to the molecules and system studied, such errors can be minimized if the systems are conditioned with the appropriate parameters and algorithms.

The objective of this project will be to determine the macroscopic properties such as density, surface tension and interfacial tension, by using molecular dynamics simulation in two-phase systems: liquid-gas and liquid-liquid, with the LAMMPS program.



Representation with VMD of MD simulations using LAMMPS of density and interfacial tension of liquid-liquid and liquid-gas systems respectively.

This work will measure the interfacial tension between liquid-liquid and liquid-vapor systems between water and the following organic compounds: benzene, nitrobenzene, hexane, ethanethiol, perfluoro-2-methylpentane at 25ºC and at 1 atm.

Finally, a bibliographic search will also be made, to look for experimental data results of each simulation done, using the Reaxys database, comparing afterwards the results obtained in each simulation with the experimental ones.

Keywords interfacial tension, superficial tension, molecular dynamics simulation, Reaxys, LAMMPS.