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Simulation methods and molecular interactions: Challenges and opportunities

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Abstract

Nowadays, the computer simulation methods are powerful tools to understand and to predict the macroscopic properties of matter from molecular interactions.

The trajectory of molecules in a molecular dynamics are generated by solving Newton´s equations of motions coupled to thermostat and barostats. In this talk I will describe methods to develop effcient algorithms of molecular dynamics simulations by using the Liouville formalism of clasical mechanics. The force field parameters are the key ingredients to be able to reproduce the experimental information. I will evaluate and discuss the weaknesses of well known force fields such as TraPPE-UA, OPLS/AA and CHARMM in simulations of liquids with several components and phases. I will present a new strategy, that include electronic structure calculations, to develop force fields that improve the agreement with experimental data. Applications will cover the use of cocrystals and ionic liquids to increase solubility of drugs in water and the simulation of solvents that are used in lithium ion batteries to storage energy.

Short bio

I am a full professor of Chemistry at the Universidad Autónoma Metropolitana-Iztapalapa since 1984. Several undergraduate and graduate students have been obtained their degree under my supervision. I am expert in developping and applying molecular simulation methods such as Brownian dynamics, molecular dynamics, Monte Carlo and dissipative particle dynamics. I have published 86 scientific articles in international journals. Those works have around 4000 citations according to Google Scholar. The highly massive parallel molecular dynamics programs GROMACS (Holland) and LAMMPS (USA), widely used word wide, has implemented one of our algorithms to couple temperature and pressure to the equations of motion. The program DL_MESO (United Kingdom) also implemented our method to include coulombic interactions in mesoscopic simulations.

My research simulation work is oriented to study problems of technological interest in fields such as energy storage, development of drugs and organic solvents; and separation of oil contaminants. The study involves the improvement of the current force field by using electronic structure and molecular dynamics calculations. A systematic procedure to improve the force fields of polar liquids have been developped in my group.