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Force field in molecular simulations, limitations, applications and perspectives in different areas of science

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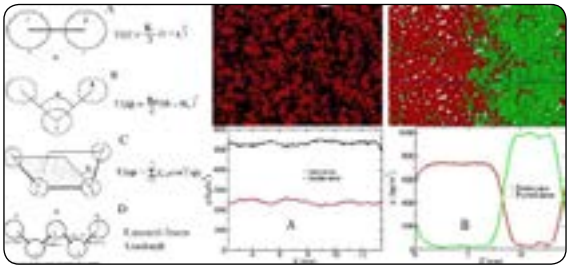
Physical properties of a molecular system are function of the interaction among molecules and atoms which form such system. These interactions are divided in two kinds, intramolecular and intermolecular. Intramolecular interactions describe the energetic contribution due to the interactions within the molecular structure, namely, bonds, angle bonds and torsions mainly; functions used for these interactions are harmonic potentials- a special mathematical models for the dihedral angle. Intermolecular potentials describe the energetic contribution of the interaction between atoms which belong to different molecules in a system, they are modeled with Lennard-Jones and Coulombic potential. In molecular simulations, the force field is essential. It is a mathematical function which includes all the energetic contributions mentioned above. Also, the force field is the set of parameters required for all the terms of the mentioned function (force constants for the harmonic, constants for the functions of the torsions, equilibrium distances and angles, Lennard-Jones parameters and electrical charges, etc.). Understanding the force field and its development has allowed the description, with some limitations, of the physical behavior of molecular systems and therefore, giving a predictive character to this methodology.



Recent Publications

1. F J Salas et al. (2015) Systematic procedure to parametrize force fields for molecular fluids. Journal of Chemical Theory and Computation 11(2):683-693.
2. AP de la Luz et al. (2015) A new force field of formamide and the effect of the dielectric constant on miscibility. Journal of Chemical Theory and Computation.11(6):2792-2800.
3. E Núñez Rojas et al. (2017) Molecular dynamics simulations to separate benzene from hydrocarbons using polar and ionic liquid solvents. Journal of Molecular Liquids. 249:591-599.
4. F J Salas, E Núñez Rojas and J Alejandre (2017) Stability of formic acid/pyridine and isonicotinamide/formamide cocrystals by molecular dynamics simulations. Theoretical Chemistry Accounts. 136(1):17.
5. E Núñez Rojas et al. (2018) Force field benchmark of the TraPPE UA for polar liquids: density, heat of vaporization, dielectric constant, surface tension, volumetric expansion coefficient and isothermal compressibility. The Journal of Physical Chemistry B. 122(5):16669-1678.

Biography

Edgar Núñez Rojas has received Degree in Chemical Engineering, UNAM School of Chemistry, Master of Science in Materials Engineering, UNAM Materials Research Institute, Doctorate in Materials Science and Engineering, Materials Research Institute UNAM, two years of postdoctoral stay at the UAM-Iztapalapa , eleven years as a subject teacher at the Faculty of Chemistry, UNAM. Two quarters as a tenured professor level C at the UAM-Iztapalapa. He currently works at the UAM-Iztapalapa as the CONACyT Chair in the Chemistry Department.

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