Force field in Molecular Simulations, limitations, applications and perspectives in various areas of knowledge

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The physical properties of any molecular system depend on the interaction of the atoms and molecules that make up these systems. These interactions can be divided into two large groups, intramolecular and intermolecular. The first ones are those that describe the energetic contribution due to the atoms contained in the molecule, that is, the bonds, the bond-angles and torsions. Intermolecular interactions describe the way in which atoms of different molecules interact and they are described by potentials of the Lennard-Jones type and by the electrostatic potential.

In the field of molecular simulations, the force field is an essential part. It is a mathematical function that includes all the energetic contributions of the mentioned interactions. Also, the force field is the set of parameters necessary to calculate energy due to all contributions mentioned (constants of harmonic potentials, cosine functions, distances, equilibrium angles, etc.).

The understanding of the force field and its development have allowed to describe, with some limitations, correctly the physical behavior of the systems and, therefore, give a predictive character to the molecular simulations.