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Structure-Force Field Generator for Molecular Dynamics Simulations

Carlos M. Patiño
Department of Physics, Universidad de los Andes
Lorena Alzate and Alejandro Strachan
School of Materials Engineering, Purdue University

ABSTRACT

Atomistic and molecular simulations have become an important research field due to the progress made in computer performance and the necessity of new and improved materials. Despite this, first principle simulations of large molecules are still not possible because the high computational time and resources required. Other methods, such as molecular dynamics, allow the simplification of calculations by defining energy terms to describe multiple atom interactions without compromising accuracy significantly. A group of these energy terms is called a force field, and each force field has its own descriptions and parameters. The objective of this project was to develop a nanoHUB tool that allowed the calculation of all the force field parameters required to perform molecular dynamics simulations in polymers and molecular systems using a widely used software called Large scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). The tool is written in Python 2.7 using OpenBabel and LAMMPS libraries, and it is currently implemented for generating DREIDING parameters and atomic charges with two methods: Gasteiger and Qeq. The LAMMPS Structure Generator takes an input file containing the atom positions in any system and format supported by OpenBabel and outputs a file with all the additional parameters required to run a simulation in LAMMPS using DREIDING force field. This software allows any researcher to run a simulation of polymers or molecules with an input file created immediately and for free.

KEYWORDS

Materials Science, Modeling, Polymers, Force Field, LAMMPS, nanoHUB