FireCore for modeling of self-assembling organic molecules on ionic substrates

Milan Koci, Prokop Hapala, Paolo Nicolini

Institute of Physics, Czech academy of Sciences, Prague, Czech Republic

The development of molecular nanotechnology hinges on our ability to predictably assemble molecular components in complex supramolecular structures. While atomic force microscopy (AFM) manipulation is an invaluable tool for prototyping molecular nanomachines, mass production requires deterministic self-assembly of simple building blocks. Atomistic simulations are crucial for developing reliable self-assemblers and nanomanipulation protocols, but they are hindered by the exponential increase in complexity of configuration space with the rising number of soft degrees of freedom, which complicates exhaustive exploration. To address this, we present a specialized classical force field (CFF) simulation package, FireCore (https://github.com/ProkopHapala/FireCore), tailored for flexible organic molecules interacting noncovalently with rigid substrates or AFM tips.

Unlike other CFF programs, FireCore is capable of leveraging massively parallel graphics processing units (GPUs) to accelerate simulations of small systems (<1000 atoms), by parallelization over many replicas of the same system. In addition, interaction of molecules with rigid substrates is accelerated by interpolation of grid projected non-covalent force-field (GridFF). Combination of all these techniques allows us to sample up to million molecular configurations per second on a single GPU accelerated workstation.
We will also introduce ongoing research focusing on rapid and efficient representation of molecular configurations, and evaluation of their similarity, which is a prerequisite for implementation of advanced global optimization and free energy sampling algorithms. This includes multi-level comparison, based on rotationally invariant descriptors such as principal axis, distribution of atomic species, as well as spatial hashing.