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Validation of the chitin parameterization in the OPLS force field

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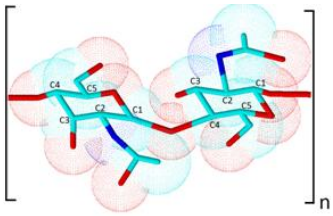
Abstract: The computational parameterization of the biopolymer chitin in the OPLS (Optimized Potentials for Liquid Simulations) force field is done, this work is essential for the theoretical study in what refers to the analysis of all the atoms present in the system, mainly to the atoms of hydrogen.

Chitin (CHT) is a very versatile biopolymer and most often used as an adsorbent decontaminant in water, Figure 1.

Figure 1: a- Three-dimensional representation of the chitin dimers and their respective van der Waals surfaces, with the nomenclature of the carbon atoms of the glycosidic chains, n being the degree of polymerization. **b-** Three-dimensional representation of 3 monomers of chitin used to perform the parameterization of this work.



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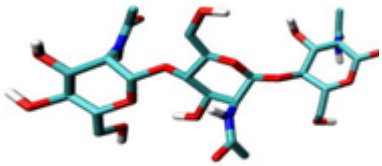
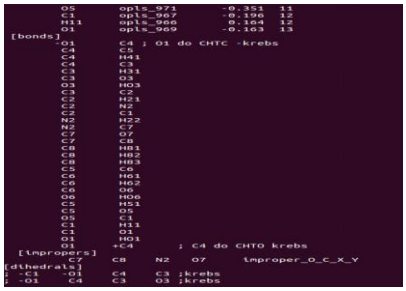


b-

The CHT were parameterized previously in force field GROMOS54a7 in GROMACS computational package and obtained excellent results, but the present research group assembled the new parameters to simulate chitin also in the OPLS-AA, where the behavior of all the atoms of the system can be analyzed.

The determination of the chitin RESP (Restrained Electrostatic Potential) is fundamental for refined parametrization. Some charges obtained are shown in Figure 2. It was noticed that atoms of the same element had different charges, this is due to the chemical environment in which the atoms were immersed. During the procedure of obtaining the RESP were fixed in order to eliminate the errors of calculations. The quantum methodology used in the load calculations was 6-31G *.

Figure 2: Charge obtained for the chitin.



After finalization of the parameterization, a molecular dynamics simulation was performed as a way to validate the parameters inserted in the force field. The simulation time was 50 nanoseconds (ns) ou 50000 picoseconds (ps). For possible property predictions the root mean square deviation in structure of CHT was calculated, to analyze the distances between the atoms of CHT and the total energy of the system containing a chitin trimer in vacuo (Figures 3 and 4, respectively).

Figure 3: RMSD for CHT.

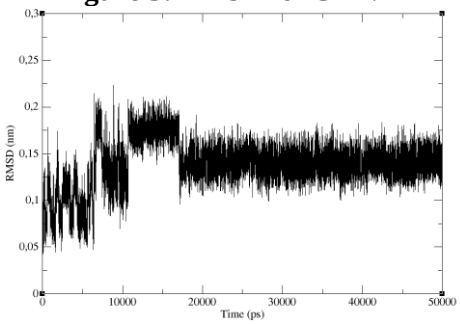
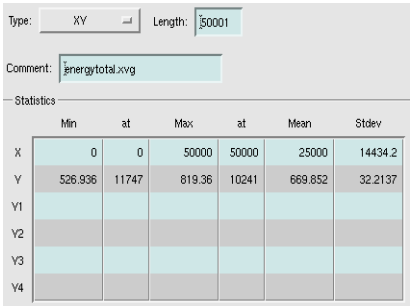


Figure 4: Table with total system energy data.



The state of the art of molecular dynamics validated the RESP obtained in the chitin parameterization performed for the OPLSAA force field, and the system and rmsd energy data show that the system converged to the termidamic equilibrium in time of approximately 16ns.

Key-words: parametrization; chitin; resp; oplsaa

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