# Molecular Dynamics Simulation of Poly(vinylidene fluoride)

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Polymers are materials with outstanding properties and a wide range of applications that originate from their macromolecular character and the diversity in their chemical structure and molecular architecture. Poly(vinylidene fluoride) (PVDF) is a highly non-reactive, thermoplastic polymer that is produced by the polymerization of 1,1- difluoroethylene. PVDF is an easy-to-process polymer, as it is soluble in a wide variety of solvents. It has very good mechanical properties, chemical resistance to oxidizing agents and high thermal stability. Due to its good barrier properties, this polymer is used in many cutting – edge technological and industrial areas [1] as a novel separation media in desalination and in the protection of materials from gas or liquid contamination. Fundamental understanding of the structure-property relationship of materials is essential to enable the design of advanced products and processes from the molecular level. Molecular simulation is a particularly efficient and reliable tool in the study of molecular mechanisms, the design of new materials and the prediction of their properties.

This work involves the study of amorphous, bulk PVDF systems via atomistic simulations using a classical all-atom force field [2] that has been further optimized. This work involves the study amorphous, bulk PVDF systems via atomistic simulations using a classical all-atom force field [2] has been further optimized. Very long molecular dynamics simulations have been performed at various statistical ensembles (NVT, NPT, NVE) and a wide range of properties (thermodynamic, structural, dynamical) have been calculated. The effect of temperature has been studied by conducting simulations at 450K, which is close to the melting point of PVDF and at 493 K. The influence of the molecular weight on the extracted properties has been thoroughly investigated by simulating several molecular weight systems between 1300 and 26000 g/mol. The systems microscopic characteristics were extracted by calculating the radius of gyration, radial distribution functions, and the characteristic ratio. The local dynamics and the relaxation times of the systems' various modes of motion were quantified by autocorrelation functions of various vectors (e.g. end-to end and bond vectors and dihedrals). The present work is the basis for subsequent research that involves the implementation of computational methods [3] for the study of the permeability and selectivity properties of PVDF and PVDF-based composites to small molecules, focusing in $CO_2$ capture and separation.

References

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