

# Eco-Design of Packaging Commodity Polymers by Validated Multiscale Modelling

## MICINN Project 2020-2023

Among the extensive number of plastic applications, **the multilayer plastic packaging** has reached a significant impact in preserving food and beverages. **Multilayered films are composed of different commodity polymers, stacked in one sheet to improve their functionality.** The typical multilayer film used in packaging is composed of three polymer layers providing mainly mechanical stability, adhesion and barrier properties (oxygen and moisture protection), respectively.

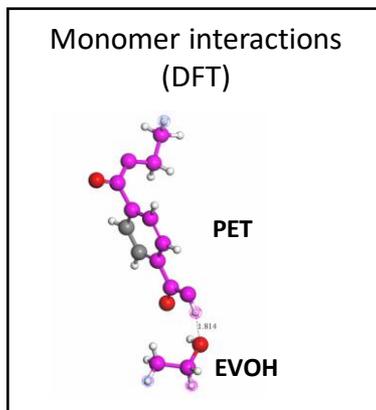
To minimize environmental injury, mechanical recycling of plastic films has reached a great relevance as an alternative route. However, **it has been proved that the chance to recycle these products can only be economically viable if recycling is taken into account during the design of packaging materials.** Thus, a key aspect for an appropriate recycling will be a better design of the plastic components based on polymer commodities using the eco-design paradigm.

The ultimate goal of this project is the **understanding of the interactions between the polymeric components usually found in multilayer films used in packaging by means of multiscale modeling** at different length-time scales. In parallel, targeted experiments will be carried out to accomplish the verification and validation of the computational models.

**Keywords:** Multiscale modeling, eco-design, packaging, mechanical recycling

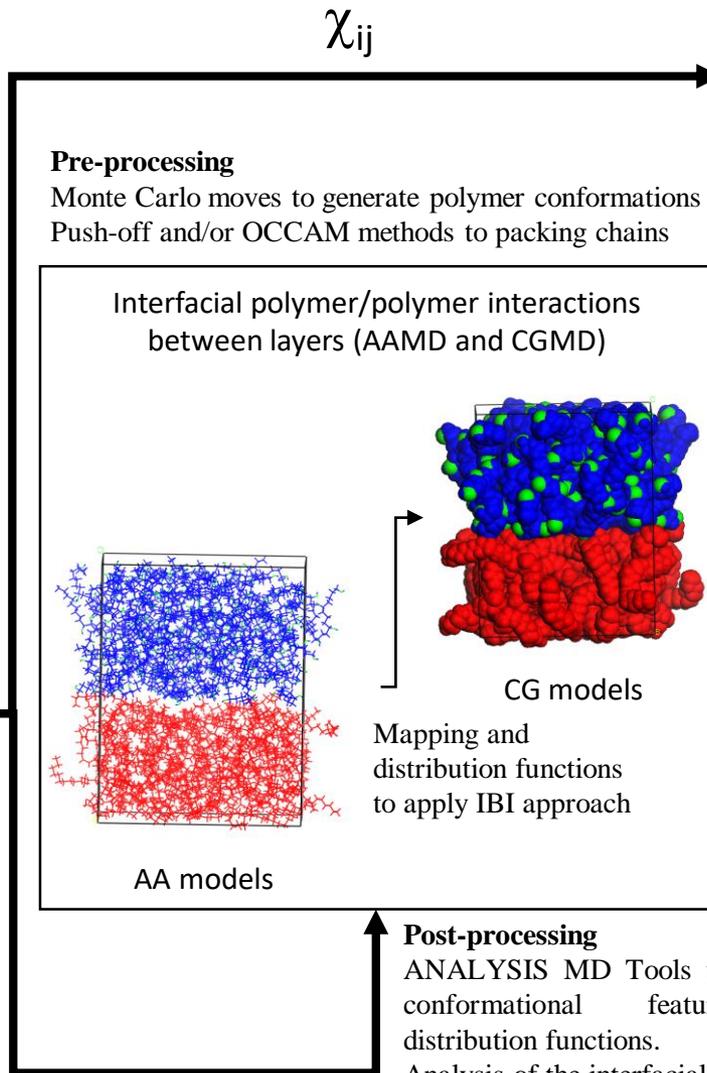
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**Pre-processing**  
CHIRIPA Tool to generate the monomer pairs using a MC algorithm



**Post-processing**  
CHIRIPA Tool to analyze and calculate  $\chi_{ij}$  and Z from the DFT calculations.

**Experimental validation**  
FTIR, NMR and melting-depression temperature

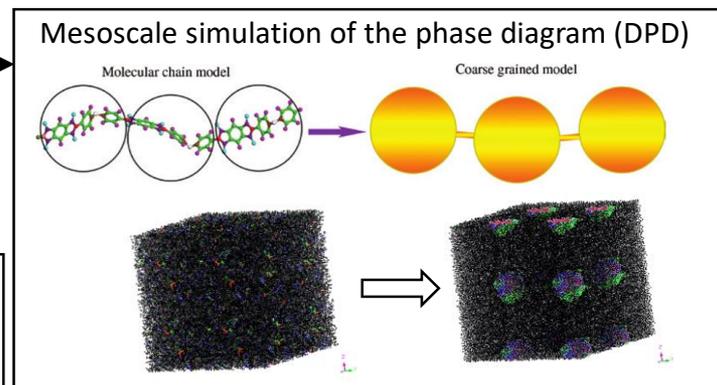


**Data to refine force fields**

**Pre-processing**

Software to map the parameters from DFT and AAMD simulations.

Generation of initial coordinates



**Conformational features and stiffness of polymer chains from their chemical structure**

**Post-processing**

Software to analysis the thermodynamics phases

**Experimental validation**  
AFM, TEM, Rheology experiments

**Post-processing**  
ANALYSIS MD Tools to calculate conformational features and distribution functions.

Analysis of the interfacial properties

**Experimental validation**  
Rheology and peel experiments

