RETASTE Conference Abstracts
Vol. 1 RETASTE-UTL-55
Athens, Greece, 6-8 May, 2021

Prediction of Properties of Poly(L-lactic acid) with the Aid of Atomistic Molecular Dynamics Simulations

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Abstract

We present results of Molecular Dynamics simulations of L-poly(lactic acid) in the context of modelling and optimising its synthesis from recyclable food waste material. Predicted properties will serve both as input for the optimisation of the synthesis process and as benchmark for the pilot plant. A fully atomistic force field from the relevant literature (McAliley & Bruce, 2011) has been utilised to simulate amorphous and crystalline structures of isotactic L-PLA of various molecular weights from decamer to 100-mer. The structures have been relaxed and subsequently simulated at the isothermal-isobaric ensemble at atmospheric pressure and temperatures from 200 degrees Celsius down to ambient conditions, covering a range between conditions of PLA synthesis and those of end-product usage, respectively. Predictions include structural (static structure factor, radius of gyration), dynamic (decorrelation time scales), transport (self-diffusion, viscosity) and thermodynamic (density, isothermal compressibility) properties as functions of PLA molecular weight. The glass transition temperature has also been verified by gradually lowering the temperature below the above mentioned range and looking at the change in slope of specific volume with temperature. Finally, the Young modulus has been predicted by looking at the change in energy with elongation of the simulated cells. Where experimental data are available, predicted properties are in very good agreement.

Keywords: polylactic acid, molecular simulation, molecular dynamics, bioplastic

References

McAliley, J.H. and Bruce, D.A., 2011. Development of force field parameters for molecular simulation of polylactide. Journal of chemical theory and computation, 7(11), pp.3756-3767.

Acknowledgments: This research has been co-financed by the European Union and Greek national funds through the Operational Program Competitiveness, Entrepreneurship and Innovation, under the call RESEARCH–CREATE–INNOVATE (project code:T1EDK- 02746)