

Polymer Informatics Tools for Sustainable Practices

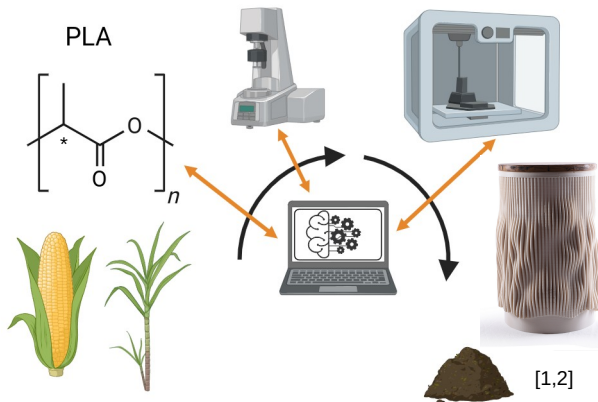
Petra Bačová, Eleftherios Christofi, Vagelis Harmandaris,
Sergio I. Molina

Departamento de Ciencia de los Materiales e Ingeniería Metalúrgica y Química
Inorgánica, Facultad de Ciencias, IMEYMAT, Campus Universitario Río San Pedro
s/n., Puerto Real, Cádiz 11510, Spain



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[1] <https://adicork.es/index.php/sectores/>; [2] Created with BioRender.com



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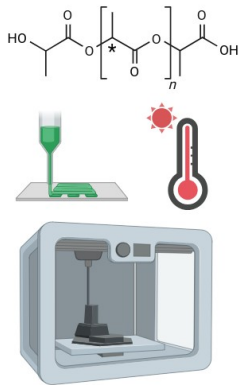


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Poly(lactic acid) in additive manufacturing

- ✓ widely popular, easy to print
- ✓ low melting point, no heated tray
- ✗ sensitive to sunlight and high temperatures
- ✗ commercial samples of unknown composition
 - L- vs. D- stereoisomer
 - additives, polydisperse samples
 - empirical approach to nanocomposite design



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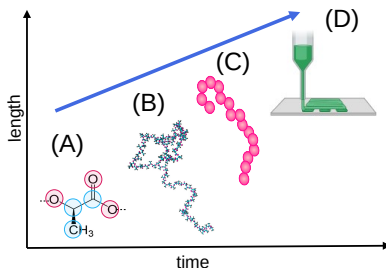
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Systematic bottom-up simulation approach

Computational methods:

- (A) quantum: force field
- (B) atomistic:
chemistry-specific
interactions
- (C) coarse-grained: trends at
mesoscale
- (D) continuum

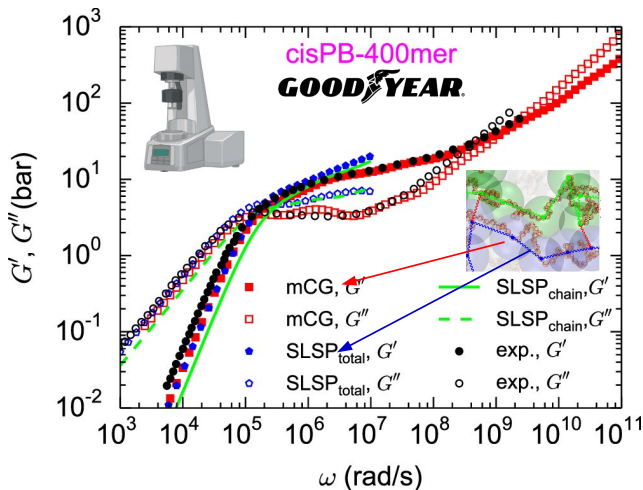


Multiscale:

- ✓ quantitative predictions of macroscopic properties
- ✗ time and resource intensive

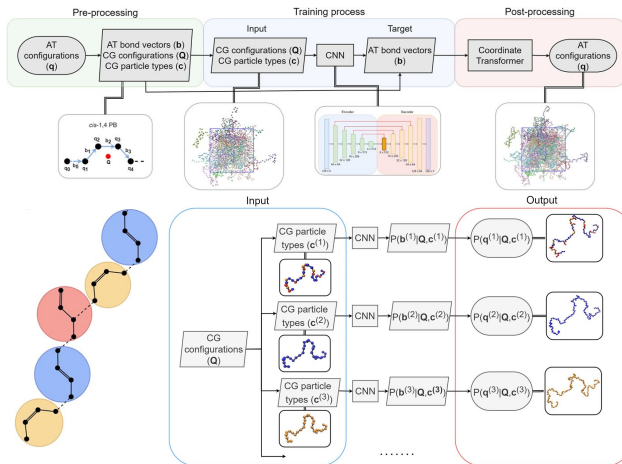
[1] Guseva, D. V.; Glagolev, M. K.; Lazutin, A. A.; Vasilevskaya, V. V.; Polym. Rev. 2023, 0, 1–39

Computer design: reproducing experiment



A. F. Behbahani et al., Macromolecules 2021 54 (6), 2740-2762

Computer design: backmapping strategy



Eleftherios Christofi et al., J. Chem. Phys. 2022 157 (18), 184903



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Challenges and motivation

- ✗ biodegradable polymers similar to proteins: **slow** structural rearrangements
- ✗ H-bonds: **atomistic detail**
- ✗ chirality: **random** L- and D- content
- ✗ lack of **open-access data** for data-driven approaches
- ✓ extensive atomistic data set which can be used for systematic bottom-up and/or data-driven approaches
- ✗ lack of experimental reference, **monodisperse and well-defined** systems
- ✓ theoretical and experimental rheological data on reference systems to determine printability



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Systems under investigation

- ▶ molecular dynamics simulations: atomistic and coarse-grained
- ▶ non-entangled melts
- ▶ 500K, 1 atm

Label	Mw [g/mol]	Microstructure	
		<i>PLLA</i>	<i>PDLA</i>
PLLA100	7.2 k	100%	0%
PDLA100	7.2 k	0%	100%
Copo100	7.2 k	45%	55%
PLLA30	2.2 k	100%	0%
PDLA30	2.2 k	0%	100%
Copo30	2.2 k	84%	16%



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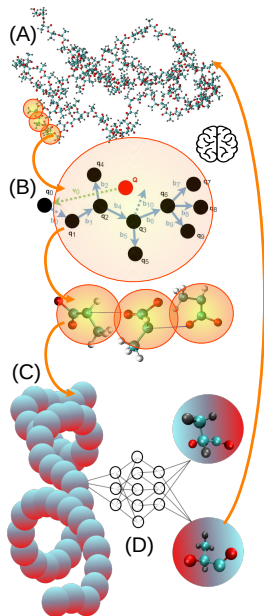


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Backmapping procedure

- (A) atomistic dataset, 5000 frames per system, training set: PLLA100, PDLA100 and Copo100
- (B) encoding and learning
 - convolutional neural network
 - versatile: bond vectors and lengths
 - local: no intermonomeric and intermolecular information
- (C) coarse-graining, monomer-like representation
- (D) backmapping
 - verify the model
 - testing the transferability



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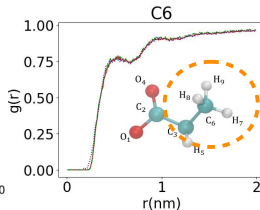
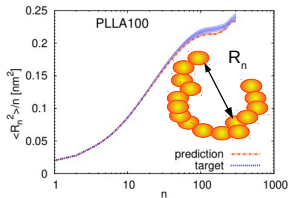
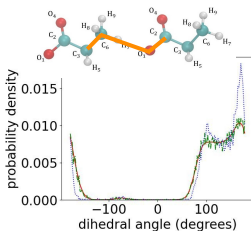
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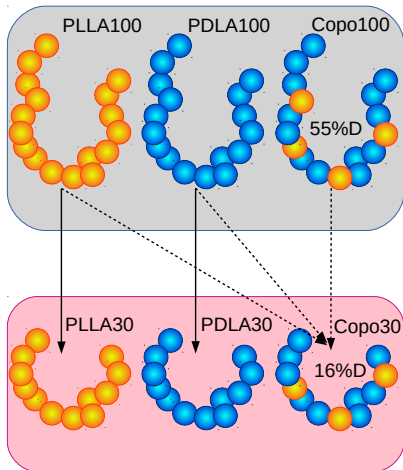
Backmapping procedure: verifying the model

- ▶ loss functions
- ▶ reproduction of the correct stereochemistry: percentage of the chiral centers with misplaced hydrogens
- ▶ polymer structure in melt
 - ➔ intramolecular: dihedral angles, intramolecular packing, characteristic ratio
 - ➔ intermolecular: intermolecular packing, density



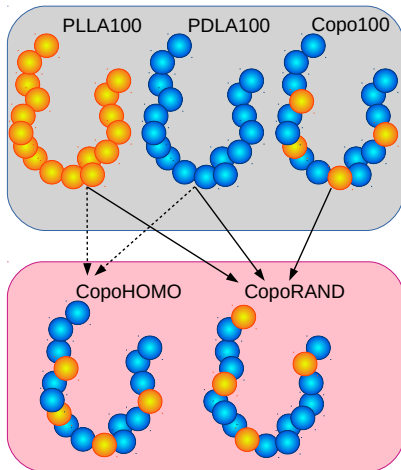
Backmapping procedure: transferability across Mw

- ▶ training set: PLLA100, PDLA100 and Copo100
- ▶ transferability across Mw: PLLA30, PDLA30, Copo30
- ✓ possible extension to any molecular weight: **industrially relevant Mw, polydisperse samples**



Backmapping procedure: chemical transferability

- ▶ training set: PLLA100, PDLA100 and Copo100
- ▶ chemical transferability
 - ➔ copolymer with a different copolymer sequence
 - ➔ copolymer trained solely on homopolymers
- ✓ capability of creating any composition: **mimicking conditions during synthesis**



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Keep calm and stay tuned!

✉ petra.bacova@uca.es

👉 <https://polysim.eu/>

👉 PITS3D project (Grant agreement ID: 101105208):
<https://cordis.europa.eu/project/id/101105208>

📖 Eleftherios Christofi, Petra Bačová, and Vagelis A. Harmandaris, Journal of Chemical Information and Modeling 2024 64 (6), 1853-1867:
<https://pubs.acs.org/doi/10.1021/acs.jcim.3c01870>



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