# Computational Modeling of Polymer Materials

**Petra Bacova**[1#*], **Eirini Gkolfi**[2] and **Vagelis Harmandaris**[1,2]

[1] Institute of Applied and Computational Mathematics, Foundation for Research and Technology Hellas, Heraklion Crete, Greece

[2] Department of Mathematics and Applied Mathematics, University of Crete, Heraklion Crete, Greece

# Presenting author: Petra Bakova, email: pbakova@iacm.forth.gr

* Corresponding author: Petra Bakova, email: pbakova@iacm.forth.gr

## ABSTRACT

We design novel polymer materials by means of atomistic molecular dynamics simulations. We focus on various types of star-shaped polymers, which are promising candidates for the realization of new emerging applications, as for example energy storage. The used computational method allows us to describe chemical details of the material and thus to mimic the behavior of the polymer structures, whose synthesis in real lab conditions is a very time-consuming task.