#### ΠΑΝΕΠΙΣΤΗΜΙΟ ΚΡΗΤΗΣ ΤΜΗΜΑ ΕΠΙΣΤΗΜΗΣ ΚΑΙ ΤΕΧΝΟΛΟΓΙΑΣ ΥΛΙΚΩΝ

#### ΠΑΡΟΥΣΙΑΣΗ ΔΙΠΛΩΜΑΤΟΣ ΜΕΤΑΠΤΥΧΙΑΚΩΝ ΣΠΟΥΔΩΝ

## Τίτλος

# «Viscoelastic properties of supramolecular gels based on hydrogen bonding»

# «Ιξωδοελαστικές ιδιότητες υπερμοριακών γελών με βάση δεσμούς υδρογόνου»

του Εμμανουήλ Βερερουδάκη μεταπτυχιακού φοιτητή του

Τμήματος Επιστήμης και Τεχνολογίας Υλικών, Πανεπιστημίου Κρήτης

Επιβλέπων καθηγητής κ. Δημήτριος Βλασσόπουλος

Τρίτη 13/07/2020

### 16:00

### https://teleconf.materials.uoc.gr/b/sta-pah-dkw

Η παρουσίαση θα διεξαχθεί με τηλεδιάσκεψη στον παραπάνω σύνδεσμο, σύμφωνα με α) την παρ. 1 του άρθρ.12 της από 11.3.2020 Πράξης Νομοθετικού Περιεχομένου (Α'55), και τις οδηγίες εφαρμογής Α Δ1α/Γποικ.28237/5.5.2020 Κ.Υ.Α (Β'1699), ΑΔΑ: ΨΠ7046ΜΤΛΗ-43Φ.

Περίληψη:

Understanding the self-assembly of supramolecular moieties and how it is affected by the presence of competitive associations is a challenging subject with potential implications on biological function. From the standpoint of materials physics, the interest lies in the fact that once the repercussions of these competitive interactions are understood, one can design materials with tunable structure or properties. There are various systems, aqueous or in organic solvents in which those interactions lead to unexpected results. Recently, it has been found that the self-assembly of supramolecular moieties in organic solvents is affected by the presence of trace amounts of water in the monomeric state that induce competitive association and change the helicity of the assembled structure. Associations between different supramolecular gelators have been known to affect the viscoelasticity of gels, by augmenting the mechanical properties or altering the dynamics. In this work, we consider two different systems, one in dodecane which is the system sensitive to humidity (BPTA) and another in water which is the mixture of a

supramolecular gelator (BTA) with a telechelic polyethylene glycol chain with the ends functionalized with BTA (BTA-PEG-BTA). We study them with a combination of rheology, microscopy and molecular dynamics simulations. In the BPTA system, water content affects the self-assembled structure by changing the persistence length and contour length of the fiber. The content of water in the fiber changes with temperature, bequeathing the viscoelastic properties with unusual temperature responsiveness. As the temperature increases from 15 to 35 °C, the relaxation time of the system varies non-monotonically with temperature. This stems from the fact that the system seems to lose its reversible and dynamic character for temperatures above 35 °C where water does not mediate the association of BPTA units. This system is studied with a combination of rheology and light scattering and this phenomenon is discussed in the context of water content of the fiber and the changing structure of the fiber. On the other hand, the mechanical properties of the water-based system exhibit non-monotonic behavior with mixing ratio, showing a maximum at 1:1 mixing ratio. However, the interactions between the two monomers (BTA and BTA-PEG-BTA) affect the self-assembly of the supramolecular polymers due to the different associating strengths of the monomers, making the fibers in the mixtures much shorter compared to the fibers created in the pure BTA network. A coarse-grained model only using the difference in the association strength of the two units can qualitatively capture the nonmonotonicity of the mechanical properties potentially providing ingredients for design of tailorable hydrogels for use in biomedical applications.