Theoretical and Physical Chemistry Institute

National Hellenic Research Foundation

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LECTURE

"Simulations in polymer networks, nanocomposites and scaffolds"

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Thursday, February 1, 2024, 12:00

Seminar room, ground floor, NHRF

Simulations in polymer networks, nanocomposites and scaffolds

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The subject of the present seminar is the detailed investigation of structural, mechanical, topological and local-segmental properties of epoxy networks of different crosslinking degrees, as well as of interfaces between these networks and graphenic (inclusion) materials. Using atomistic simulations as the principal tool, an epoxy in the bulk is first studied. Following that, the thermodynamics, structure, and interfacial kinetics of a nanocomposite consisting of parallel single layers of pristine, defective, or chemically modified graphene enclosed in the epoxy are investigated.

The study of the nanocomposite interface is targeted at the failure of adhesion brought about by imposition of shear deformation. A new methodology is developed which extends the Boltzmann-Arrhenius-Zhurkov model and it is applied in the prediction of the mechanical response of the material under shear stress. Testing the methodology for the three types of graphenic and carbon nanotube inclusions over a wide variety of temperatures and stresses, favorable agreement with experimental studies is observed and the factors controlling adhesion at the interface are elucidated.

At the end, results from the mechanical characterization of 3D printed scaffolds from hybrid nanocomposites, with specific geometry, they will be presented, focusing on bone regeneration applications.