**NATIONAL TECHNICAL UNIVERSITY OF ATHENS**
**SCHOOL OF CHEMICAL ENGINEERING**
**Department of Materials Science and Engineering**
**Computational Materials Science and Engineering (CoMSE) Group**

# Post-doctoral position available

A new post-doctoral researcher position is available in the CoMSE Group at NTUA in the context of the research programme "Multiscale Simulations of Complex Polymer Systems" (MuSiComPS), carried out in collaboration with the University of Patras thanks to the generous support of the Limmat Foundation, Zurich, Switzerland. The new position is available immediately (starting date 1 March 2015) for one year, with the possibility of extension for two additional years. The gross salary will be 35,000 €/yr.

The project to be undertaken by the post-doctoral researcher is outlined below.

Candidates holding a Ph.D. in Chemical Engineering, Materials Science and Engineering, or any other branch of Engineering, in Physics, or in Chemistry, with an excellent academic record, a strong background in molecular and multiscale modelling, extensive experience and demonstrated talent in large-scale computational research are encouraged to apply by sending a curriculum vitae and arranging for two letters of recommendation to be e-mailed directly to

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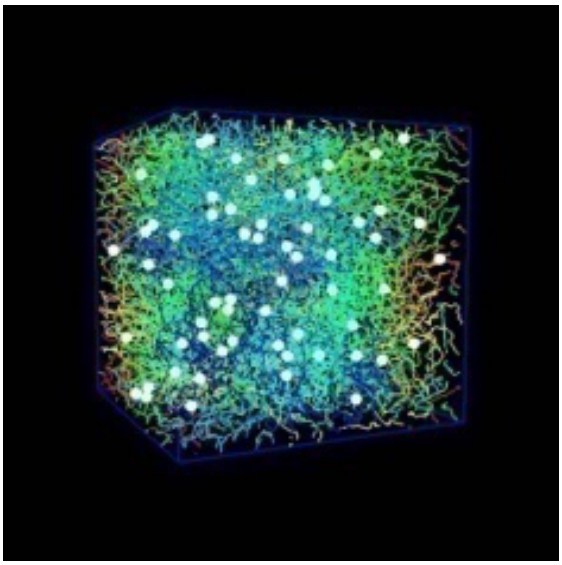
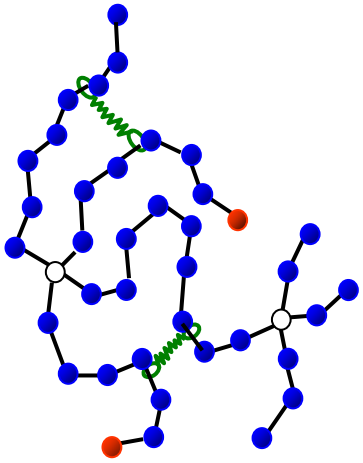
**Position NTUAPostDoc: Atomistic and mesoscopic simulations of the viscoelastic properties of elastomeric networks (NETWORKS)**





Crosslinked polymer networks, either neat or swollen with solvent, are ubiquitous in nature and technology. Physically or chemically crosslinked amorphous polymer networks above their glass temperature exhibit rubber elasticity, being capable of stretching by several hundred percent and essentially recovering their original dimensions upon release of the stress. They find use in items ranging from rubber bands to heart valves and gaskets in supersonic jet planes and, when filled with nanoparticles such as carbon black or silica, are valuable as tire materials.

In this project, atomistic and mesoscopic simulations of elastomeric networks will be undertaken in order to predict their frequency-dependent mechanical response as a function of their molecular characteristics. Networks of simple polyolefinic (e.g. ethylene-propylene rubbers or EPMs) or polydienic (e.g. cis-1,4 polyisoprene or natural rubber) chemical constitution will be considered. A coarse-grained bead-and-spring representation with crosslinks and slip-links representing entanglements will be parameterized on the basis of detailed atomistic simulations, validated for networks amenable to both atomistic and mesoscopic analysis, and used to predict the mechanical response of more complex systems with long relaxation times.

The project will involve (i) prediction of the stress-strain relation under uniaxial tension; (ii) computation of linear viscoelastic functions; (iii) investigation of the role of network topology on properties; (iv) large amplitude oscillatory shear experiments and analysis of the concomitant nonlinear response.