



## Wolfson Department of Chemical Engineering Graduate Seminars

Lecture Hall 6, Wolfson Department of Chemical Engineering, **March 16, 2016, Wednesday, 13:30**

### **Riki Klein**

M.Sc student, supervisor Prof. Simcha Srebnik

## **Molecular modeling and investigating of thermo-mechanical properties of epoxy resin using molecular dynamics simulation**

Epoxy resins are important thermosetting polymers in industry. They display a unique set of properties and are available in a wide variety of forms, which makes them suitable for different application and processes. They are cheap, strong, have water and electrical resistance, have great adhesion to different substrates, and thus are useful as adhesives, coatings, encapsulates, casting materials, potting compounds, binders and composites. Using atomistic molecular dynamics simulation provides a cost-effective systematic procedure for evaluating properties of different systems on the macro scale as well as atomic-level detail while considering molecular changes in structure and the effect these changes have on the system's performance without conducting time consuming and high-cost experiments. We modeled crosslinking of a commercial epoxy-based resin under different degrees of crosslinking and under a range of temperatures and measured average thermodynamic and mechanical properties of the system. The calculated properties were in good agreement with experimental measurements. The model demonstrates the validity of the chosen force field and simulated crosslinking reaction, and can be used as a predictive tool for thermo-mechanical property calculation of epoxy-based resins.

### **Avishai Karny**

M.Sc student, supervisor Prof. Avi Schroeder

## **Plant-derived nanoparticles for nurturing food crops**

Nanomaterials are revolutionizing many fields, such as medicine, electronics and energy. As world population grows, there is a need for efficient and ecologically-friendly agricultural technologies to provide global food requirements. Here, we describe a plant-derived nanoparticle used to deliver nutrients and crop-protection-agents to plants. We show that 100-nm nanoparticles penetrate the leaf cuticle and travel in a bidirectional manner, distributing to the other leaves and down the roots. The particles remain intact until they internalize into the plant cells, where they release their payload. The particles are capable of carrying various compounds, depending on the need. Tomato plants treated with nanoparticles loaded with Mg and Fe overcame acute nutrient deficiency. Contrarily, to protect crops from infiltrating weeds, nanoparticles applied to Nutgrass, perturbed the leaf, penetrated the underground bulb network, and were later found in all the interlinked plant segments above ground.

To test the technological feasibility and safety, we sprayed the nanoparticles, and found they were stable for short-distance spraying (2 meters), but disintegrated into their biocompatible molecular building blocks at longer distances.

In summary, plant-derived nanotechnologies serve as new delivery platforms for crop fertilizing and protection.