



# ITE/ΕΙΧΗΜΥΘ

## ΠΡΟΣΚΕΚΛΗΜΕΝΗ ΟΜΙΛΙΑ ΠΡΟΣΚΕΚΛΗΜΕΝΗ ΟΜΙΛΙΑ

**ΟΜΙΛΗΤΗΣ:** **Dr. Nikos Benteinis**, Assistant Professor  
Department of Chemistry and Biochemistry  
Southwestern University  
Georgetown, USA

**ΥΠΕΥΘ. ΠΡΟΣΚΛΗΣΗΣ:** **Dr. Μαρία Κλάπα**, Κύρια Ερευνήτρια ITE/ΕΙΧΗΜΥΘ

**ΘΕΜΑ:** **Developing force fields from the microscopic structure of solutions:  
The Kirkwood-Buff approach.**

**ΤΟΠΟΣ:** Αίθουσα Σεμιναρίων ITE/ΕΙΧΗΜΥΘ

**ΗΜΕΡΟΜΗΝΙΑ:** **Παρασκευή, 15 Ιουλίου 2011**

**ΩΡΑ:** **12:00**

**ΠΕΡΙΛΗΨΗ:**

The talk will briefly discuss the parametrization of and the challenges with common force fields for biomolecular simulations and it will introduce the Kirkwood-Buff theory and its application to force field development. Details of the methodology will be presented and the application to the force fields of thiols, sulfides, disulfides, and benzene solutions will be explained. The application of the Kirkwood-Buff theory to the coarse-grain parametrization of a force field for an aqueous solution of an ionic liquid will be also outlined.



# ITE/EIXHMYO

## SHORT BIO

**Nikos Benteitis** is an assistant professor of Physical Chemistry in Southwestern University, in Texas. After graduating with a degree in Chemical Engineering from the National Technical University of Athens, he got his PhD under the supervision of Sonja Krause at the Rensselaer Polytechnic Institute (RPI), where he studied experimentally and theoretically the behavior polymer solutions under electric fields. He then did his postdoctoral work with Mike Shen at Colgate University, where he focused on gas electron diffraction. Nikos is currently developing both atomistic and coarse-grain force fields for biomolecules and ionic liquids.