Η Επιτροπή Σεμιναρίων της Σχολής Χημικών Μηχανικών έχει την ευχαρίστηση να σας προσκαλέσει στο επόμενο σεμινάριο της Σχολής, που θα δοθεί από τον Καθηγητή Robert Latour από το Clemson University των Η.Π.Α.

Το σεμινάριο έχει προγραμματιστεί για την Παρασκευή, 12 Ιουνίου 2009 και ώρα 13:30, στην Αίθουσα Κουμούτσου. Ο τίτλος της διάλεξης του κυρίου Latour είναι "A Parallel Tempering Algorithm for Sampling Large Molecular Systems with Replica Number Independent of System Size".

A PARALLEL TEMPERING ALGORITHM FOR SAMPLING LARGE MOLECULAR SYSTEMS WITH REPLICA NUMBER INDEPENDENT OF SYSTEM SIZE

Robert A. Latour
McQueen-Quattlebaum Professor
of Bioengineering
Clemson University
Clemson, SC, USA

While Monte Carlo (MC) and molecular dynamics (MD) simulation methods provide powerful approaches to predict the behavior of material systems at the atomistic level, conventional MC and MD simulations can be problematic because of their inability to overcome energy barriers that are greater than a few kcal/mol. This often results in a simulation being trapped in local low-energy states, thus preventing adequate system sampling and appropriate comparison of simulation results with experimentally measured values. Advance sampling algorithms, such as parallel tempering (PT), have been developed as an approach to overcome this sampling problem by using multiple replicas simulated in parallel at different temperature levels with an exchange algorithm applied to swap conformations between temperatures, thus enabling thermal energy to be used to rapidly cross energy barriers.
These methods, however, become too computationally expensive for large molecular systems (e.g., the simulation of whole proteins and protein-surface adsorption) because the number of replicas that must be used in a simulation is proportional to the number of atoms in the system. To address this problem, we have developed a new empirically based advanced sampling algorithm (TIGER2: Temperature Intervals with Global Exchange of Replicas) that has been specifically designed for the simulation of large molecular systems at low computational cost. In this presentation, I will present the development of the TIGER2 algorithm and demonstrate its application for several simple molecular systems of increasing complexity, with the sampling results compared with PT simulations for method validation.

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Δώρος Θεοδώρου