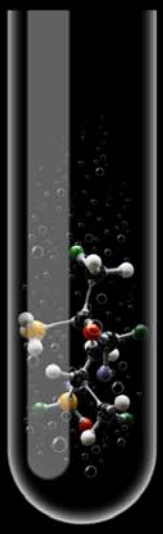

Cicle de conferències
entorn la celebració de l'any de la Química

2011

Cycloadditions: Mechanism, Dynamics, and Biological Catalysis

15-07-2011

Prof. Kendall N. Houk

Department of Chemistry and Biochemistry
University of California, Los Angeles (UCLA)

This lecture describes computational studies of 1,3-dipolar, Diels-Alder, and carbene cycloadditions using quantum mechanics and molecular dynamics. Control of reactivity through distortion and interaction energies is described. Dynamics of cycloadditions show the vibrational excitations that are necessary for reaction. Collaborations with David Baker have led to protein catalysts for a Diels-Alder reaction designed from quantum mechanical predictions of an active site and Rosetta predictions of proteins that fold with that active site.

sala de Graus de la Facultat de Ciències, 12h

UAB
Universitat Autònoma de Barcelona

2011 Any de la Química