

### Institut de Química Teòrica i Computacional de la UB

3 de juliol de 2015, Aula Enric Casassas,

Facultat de Química, Universitat de Barcelona

9:45 - 9:50	<i>Welcome</i> <b>Francesc Illas</b> , Director of IQTCUB
9:50 - 10:50	<i>"From photostability to photodamage in DNA: insights from molecular dynamics"</i> <b>Leticia González</b> (University of Vienna)
10.50 - 11:15	<i>"Adiabatic and nonadiabatic dynamics with conditional wave functions"</i> <b>Guillem Albareda</b> (IQTCUB, Universitat de Barcelona)
11:15 - 11:30	<i>"Stabilization of open-shell states in purely organic molecules"</i> <b>Daniel Reta</b> (IQTCUB, Universitat de Barcelona)
11:30 - 12:15	Coffee Break & Poster Session
12:15 - 12:40	<i>"Effect of water and coexisting impurities on the adsorption of CO<sub>2</sub> in CuBTC and zeolite 13X"</i> <b>Pablo Gamallo</b> (IQTCUB, Universitat de Barcelona)
12:40 - 13:05	<i>"Expanding the druggable genome with new computational tools"</i> <b>Xavier Barril</b> (Universitat de Barcelona)
13:05 - 13:30	<i>"Modeling the ligand tuning effect over the transition temperature in Spin-Crossover systems using Density Functional Methods"</i> <b>Jordi Cirera</b> (IQTCUB, Universitat de Barcelona)
13:30	<i>Closing</i> <b>Francesc Illas</b> , Director of IQTCUB
13:45 - open	Lunch & Poster Session