

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

30 de maig de 2014, Aula Enric Casassas,

Facultat de Química, Universitat de Barcelona

|               |                                                                                                                                                     |
|---------------|-----------------------------------------------------------------------------------------------------------------------------------------------------|
| 9:30 - 9:45   | <i>Opening</i><br><b>Jordi Alberch</b> , Vicerector de Recerca, Innovació i Transferència<br><b>Pere Ll. Cabot</b> , Degà de la Facultat de Química |
| 9:45 - 9:50   | <i>Welcome</i><br><b>Francesc Illas</b> , Director of IQTCUB                                                                                        |
| 9:50 - 10:50  | <i>"Determining Optical Spectra with Theory: an Easy Challenge?"</i><br><b>Denis Jacquemin</b> (Université de Nantes)                               |
| 10.50 - 11:15 | <i>"Spin Tricks in the Reactivity of Transition Metal Nitrene Complexes"</i><br><b>Feliu Maseras</b> (ICIQ)                                         |
| 11:15 - 11:30 | <i>"First and Second Order Phase Transitions in Dithiazolyl- based Materials"</i><br><b>Sergi Vela</b> (IQTCUB, Universitat de Barcelona)           |
| 11:30 - 12:15 | Coffee Break & Poster Session                                                                                                                       |
| 12:15 - 12:40 | <i>"Theoretical Characterization of Molecular Metal Oxides. Challenging Cases"</i><br><b>Xavier López</b> (Universitat Rovira i Virgili)            |
| 12:40 - 13:05 | <i>"Cost-Effective Catalysis on Early Transition Metal Carbides"</i><br><b>Francesc Viñes</b> (IQTCUB, Universitat de Barcelona)                    |
| 13:05 - 13:30 | <i>"Mapping Enzyme Engineering by Computational Tools"</i><br><b>Víctor Guallar</b> (ICREA, BSC-IRB)                                                |
| 13:30         | <i>Closing</i><br><b>Francesc Illas</b> , Director of IQTCUB                                                                                        |
| 13:45 - open  | Lunch & Poster Session                                                                                                                              |