



Marie Curie: IRSES

Nagoya University 



Mini Workshop

May 29, 2013 (Wed), 13:00-16:00

Chemistry Gallery, RCMS 2nd floor

Theory of Electronic Excitations in Large Molecules

Program

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| 13:00-13:05 | Opening Remarks |
| 13:05-13:35 | Frédéric Labat (CNRS, Paris): Modeling DSSCs using DFT |
| 13:35-14:05 | Diane Bousquet (CNRS, Paris): Vertical and Relaxed Excited states: DFT vs SAC-CI |
| 14:05-14:35 | Ilaria Ciofini (CNRS, Paris): Density based descriptors for excited state character and reactivity |
| 14:35-14:50 | Break |
| 14:50-15:20 | Tim Kowalczyk (Nagoya University): Static DFT methods for excited states |
| 15:20-15:50 | Daisuke Yokogawa (Nagoya University): Electronic structure calculation in solution using RISM-SCF-SEDD |
| 15:50-16:00 | Closing Remarks |



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