

Joint Seminar Hebrew University of Jerusalem – University of Vienna

“Novel Approaches in Computational Photobiology”

Fritz Haber Center for Molecular Dynamics Research, Jerusalem

1st day Wednesday, October 30th

09:00 Welcome and Introduction

09:10 *“How to run extensive excited state dynamics and survive it”*
Leticia Gonzalez (University of Vienna)

09:50 *“Laser-induced spin dynamics: Some predictions from real-time TDDFT”*
Hardy Gross (Hebrew University of Jerusalem)

10:30 Coffee break

10:50 *“Making sense of Coulomb Explosion Imaging: 2-body fragmentation”*
Ester Livshits (Hebrew University of Jerusalem)

11:20 *“Unraveling the nonequilibrium dynamics of an open system of non-interacting fermions”*
Roi Baer (Hebrew University of Jerusalem)

12:00 Lunch

14:00 *“150 years of the periodic table”*
Sason Shaik (Hebrew University of Jerusalem)

15:15 *“Stochastic basis set approach to density functional theory”*
Marcel Fabian (Hebrew University of Jerusalem)

15:45 *“Excited State Dynamics of Proteorhodopsin”*
Saumik Sen (Hebrew University of Jerusalem)

16:15 *“Porting quantum chemistry codes onto NEC's SX-Aurora vector engine - first experiences”*
Markus Oppel (University of Vienna)

16:45 Coffee break

17:05 *“Computational chemistry and organic synthesis: Let us build a bridge!”*
Boris Maryasin (University of Vienna)

17:35 *“Spectral Tuning in Cyanobacteriochrome”*
Igor Schapiro (Hebrew University of Jerusalem)

18:15 *“Nuclear quantum effects in the non-adiabatic dynamics: simple illustration in the ultrafast pumped N₂”*
Ksenia Komarova (Hebrew University of Jerusalem)

2nd day Thursday, October 31st

09:00 *"Molecular Formation in Extreme conditions"*
Tamar Stein (Hebrew University of Jerusalem)

09:40 *"Ruthenium-based complexes bound to biological lipid membranes: a computational approach"*
Pedro A. Sanchez Murcia (University of Vienna)

10:10 **Coffee break**

10:40 *"Hydrolysis of N₂O₅ using ab initio molecular dynamics"*
Estefania Rossich Molina (Hebrew University of Jerusalem)

11:10 *"Energy, Momentum and Angular Momentum Transfer Between Electrons and Nuclei"*
Chen Li (Hebrew University of Jerusalem)

12:00 **Lunch break**

14:00 *"The Many Faces of Water: An Atomistic Approach"*
Ali Hassanali (The International Center for Theoretical Physics (ICTP) in Trieste, Italy)

15:30 **Round Table Discussion**