Fritz Haber Center for Molecular Dynamics
Institute of Chemistry, The Hebrew University of Jerusalem

Beirat Symposium January 19, 2021

Organizers: Raam Uzdin and Roi Baer

Zoom link to the seminar room: https://huji.zoom.us/j/8865045794
Link for the Lounge: https://bit.ly/3nhshRm

Chair: Raam Uzdin

9:30-09:50	**Noam Agmon**, Fritz Haber Center and Institute of Chemistry, HUJI	Thermodynamics and Spectroscopy of Small Water Clusters: The Persistent Tetramer and Quantal Hexamer
09:50-10:10	**Ilan Shmulin**, Fritz Haber Center and Institute of Chemistry, HUJI (Harries group)	How Sugars Modify Caffeine Self-Association and Solubility: Resolving a Mechanism of Selective Hydrotropy
10:10-10:30	**Yigal Lahav**, Fritz Haber Center and Institute of Chemistry, HUJI (Schapiro group)	Calculating Optical Spectra of Photoresponsive Protein Complexes using QM/MM
10:30-10:50	**Helen Eisenberg**, Fritz Haber Center and Institute of Chemistry, HUJI (Stein group)	The Influence of Adsorption Geometry on Surface Catalytic Reactions
10:50-11:00	**Break in Lounge (serving number-crunching bits of cookies)**	**Link for the Lounge** https://bit.ly/3nhshRm

Opening ceremony, chair: Roi Baer

11:00-11:10	**Shlomo Yitzchaik**, Head of the Institute of Chemistry, Hebrew University of Jerusalem	Opening and welcoming address
11:10-11:30	**Gerard Meijer**, Chair of the Fritz Haber Center's Beirat, Fritz Haber Institute, Berlin, Germany	Laser-cooling and trapping AlF molecules
11:30-12:00	**Frank Neese**, Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany	TBD
12:00-12:45	**Poster Session I**	**Link for the Lounge** https://bit.ly/3nhshRm

Chair: Efrat Hadad

12:45-13:05	**Eli Kraisler**, Fritz Haber Center and Institute of Chemistry, HUJI	The exchange-correlation potential in density-functional theory: exact asymptotic behavior and strategy for advanced approximations
13:05-13:25	**Kim Asseo**, Fritz Haber Center and Institute of Biochemistry, Food Science and Nutrition, HUJI (Niv group)	Smell loss and taste loss to predict COVID-19: Google searches and self-reports
13:25-14:10	**Lunch break in Lounge (take a byte of our tasty hot meals)**	**Link for the Lounge** https://bit.ly/3nhshRm

Chair: Jon Church

14:10-14:30	**Snir Gazit**, Fritz Haber Center and Racah Institute of Physics, HUJI	Fermi surface reconstruction without symmetry breaking
14:30-14:50	**Ben Shpiro**, Fritz Haber Center and Institute of Chemistry, HUJI (Baer group)	Ab-initio Forces from stochastic DFT: a formalism in a nonorthogonal basis-set representation
14:50-15:10	**Maximilian Jakobs**, Dept. of Physiology, Development and Neuroscience, Cambridge UK (Zemel group)	Unrestrained growth of correctly oriented microtubules is crucial for establishing axonal microtubule orientation
15:10-16:00	**Poster Session II**	**Link for the Lounge** https://bit.ly/3nhshRm

Chair: Ester Livshits

16:00-16:20	**Ryan Requist**, Fritz Haber Center and Institute of Chemistry, HUJI (Gross Group)	Vector potential in the exact factorization equations and its consequences for nuclear dynamics
16:20-16:40	**Ksenia Komarova**, Fritz Haber Center and Institute of Chemistry, HUJI (Levine group)	Surprisal of a quantum state: dynamics, compact representation and coherence effects
16:40-17:00	**Natalia Karimova** Fritz Haber Center and Institute of Chemistry, HUJI (Gerber Group)	Mechanisms of the important ionic reactions at the surface of liquid water
17:00-17:15	**Coffee break in lounge (streaming steaming tea)**	**Link for the Lounge** https://bit.ly/3nhshRm

Chair: Estefanía Rossich Molina

17:15-17:35	**Vladimir Nazarov**, Fritz Haber Center, HUJI and Moscow Institute of Physics and Technology , Dolgoprudny, Russian Federation	The high frequency limit of spectroscopy
17:35-17:55	**Bar Ezra**, Fritz Haber Center and Institute of Chemistry, HUJI (Kosloff group)	Dissociation in strong field: a quantum analysis of the relation between angular momentum and angular distribution of fragments
17:55-18:15	**Ivan Henao,** Department of Physiology, Development and Neuroscience, Cambridge UK (Uzdin group)	Catalytic transformations using small quantum systems: explicit protocols and applications to cooling
18:15	**Symposium end: Good bye!**	