



# 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	<b>Noam Agmon</b> , 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	<b>Ilan Shmulin</b> , 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	<b>Yigal Lahav</b> , Fritz Haber Center and Institute of Chemistry, HUJI (Schapiro group)	Calculating Optical Spectra of Photoresponsive Protein Complexes using QM/MM
10:30-10:50	<b>Helen Eisenberg</b> , Fritz Haber Center and Institute of Chemistry, HUJI (Stein group)	The Influence of Adsorption Geometry on Surface Catalytic Reactions
10:50-11:00	<b>Break in Lounge (serving number-crunching bits of cookies)</b>	<b>Link for the Lounge</b> <a href="https://bit.ly/3nhshRm">https://bit.ly/3nhshRm</a>

## Opening ceremony, chair: Roi Baer

11:00-11:10	<b>Shlomo Yitzchaik</b> , Head of the Institute of Chemistry, Hebrew University of Jerusalem	Opening and welcoming address
11:10-11:30	<b>Gerard Meijer</b> , Chair of the Fritz Haber Center's Beirat, Fritz Haber Institute, Berlin, Germany	Laser-cooling and trapping AIF molecules
11:30-12:00	<b>Frank Neese</b> , Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany	Near accurate solutions to the many particle Schrödinger equation for systems with hundreds of atoms: opportunities and pitfalls
12:00-12:45	<b>Poster Session I</b>	<b>Link for the Lounge</b> <a href="https://bit.ly/3nhshRm">https://bit.ly/3nhshRm</a>

## Chair: Efrat Hadad

12:45-13:05	<b>Eli Kraisler</b> , 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	<b>Kim Asseo</b> , Fritz Haber Center and The Faculty of Agriculture, Food and Environment, HUJI (Niv group)	Smell loss and taste loss to predict COVID-19: Google searches and self-reports
13:25-14:10	<b>Lunch break in Lounge (take a byte of our tasty hot meals)</b>	<b>Link for the Lounge</b> <a href="https://bit.ly/3nhshRm">https://bit.ly/3nhshRm</a>



## Chair: Jonathan Church

14:10-14:30	<b>Snir Gazit</b> , Fritz Haber Center and Racah Institute of Physics, HUJI	Fermi surface reconstruction without symmetry breaking
14:30-14:50	<b>Ben Shpiro</b> , 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	<b>Maximilian Jakobs</b> , 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	<b>Poster Session II</b>	<b>Link for the Lounge</b> <a href="https://bit.ly/3nhshRm">https://bit.ly/3nhshRm</a>

## Chair: Ester Livshits

16:00-16:20	<b>Ryan Requist</b> , 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	<b>Ksenia Komarova</b> , 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	<b>Natalia Karimova</b> 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	<b>Coffee break in lounge (streaming steaming tea)</b>	<b>Link for the Lounge</b> <a href="https://bit.ly/3nhshRm">https://bit.ly/3nhshRm</a>

## Chair: Estefanía Rossich Molina

17:15-17:35	<b>Vladimir Nazarov</b> , Fritz Haber Center, HUJI and Moscow Institute of Physics and Technology , Dolgoprudny, Russian Federation	The high frequency limit of spectroscopy
17:35-17:55	<b>Bar Ezra</b> , 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	<b>Ivan Henao</b> , Department of Physiology, Development and Neuroscience, Cambridge UK (Uzdin group)	Catalytic transformations using small quantum systems: explicit protocols and applications to cooling
18:15	<b>Symposium end: Good bye!</b>	