

# Beirat Symposium Book of Abstracts



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

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# Abstracts for Invited Talks

## Thermodynamics and Spectroscopy of Small Water Clusters: The Persistent Tetramer and Quantal Hexamer

Nagaprasad Reddy Samala and Noam Agmon

19 Jan  
9:30-09:50

The Fritz Haber Center of Molecular Dynamics, The Hebrew University of Jerusalem

Small water clusters absorb heat and catalyze pivotal atmospheric reactions. Yet, experiments produced conflicting results on water cluster distribution under atmospheric conditions. Additionally, it is unclear which “phase transitions” such clusters exhibit, at what temperatures, and what are their underlying molecular mechanisms. Also of current interest is the magnitude of nuclear quantum effects (NQE) on various attributes, and how to correct classical nuclear dynamics for them. We have used the “best” overall water potential, MB-pol, which is based on many-body interactions fitted to some 5000 quantum calculations at the CCSD(T) level. We show, for the dimer to hexamer, that the cluster melting and vaporization transitions can be deduced from logarithmic tails in the radial distribution function,  $g(r)$ . The tetramer has the highest melting and vaporization temperatures, suggesting that it may live longer under atmospheric conditions. We show that the NQE are small for these properties. In contrast, the NQE is large for the IR OH stretching bands. We show that the spectra can be corrected by a temperature independent blue shift, which, however, does depend on cluster size and isomer. For the hexamer we show that the largest NQE is obtained for isomers with two-dimensional geometries, reducing as they become more three-dimensional (figure below). Figure: Spectral shifts of the OH stretch of water hexamer isomers due to NQE

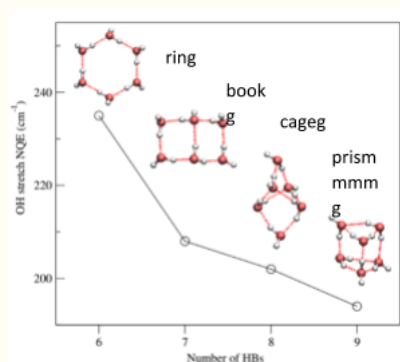


Figure 1: Spectral shifts of the OH stretch of water hexamer isomers due to NQE

19 Jan  
14:10-14:30

## How Sugars Modify Caffeine Self-Association and Solubility: Resolving a Mechanism of Selective Hydrotropy

Ilan Shumilin, Christoph Allolio, and Daniel Harries

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The aggregation of drugs and nutraceuticals in aqueous media is an outstanding problem for their efficacy and bioavailability. A common solution is to add excipients or hydrotropes that increase solubility and limit aggregation. Here we study caffeine, a widely consumed drug that undergoes oligomerization and aggregation in aqueous solutions. Combining partition and solubility experiments with molecular dynamics simulations, we determined the effect of sugars (mono- and disaccharides) on caffeine self-association and solubility. We find that sugars selectively increase the concentration of caffeine in its monomeric state, but decrease its solubility in all oligomeric forms. Thus we determine that, in contrast to common hydrotropes, sugars act as selective hydrotropes toward caffeine, since they differentially act on specific solvated forms of the drug. We furthermore unravel the molecular mechanism for this selectivity, and comment on the general design principles that should help develop targeted excipients for bioavailability and taste modification in drugs and foods.

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19 Jan  
10:10-10:30

## Calculating Optical Spectra of Photoresponsive Protein Complexes using QM/MM

Yigal Lahav<sup>1,2</sup> and Igor Schapiro<sup>1</sup>

<sup>1</sup>Fritz Haber Center for Molecular Dynamics Research, Institute of Chemistry, Hebrew University of Jerusalem, Israel.

<sup>2</sup>MIGAL – Galilee Research Institute, Kiryat Shmona, Israel.

Modelling optical spectra of protein bound chromophores can be a challenging task. The complexity of these systems prohibits the usage of vertical excitation approximation at equilibrium and requires the explicit consideration of dynamics. Over the years, ensemble-based approaches for calculating optical spectra has become widespread among the scientific community<sup>1-3</sup>. These methods provide specific description of chromophore-protein interactions but neglecting the dynamic coupling between the electronic transitions and the environmental degrees of freedom. Thus, leading to poor spectral lineshapes. Recent developments in computer hardware have opened the door for a new technique considering both dynamic coupling and pigment-protein interactions, using the cumulant expansion of the energy gap correlation function<sup>4,5</sup>, allowing the description of vibronic transitions. Thus, providing high detailed optical spectra. Here I will present the different methods, explain their difficulties, and discuss the future aspects of this work. 1 L. G. Martina De Vetta, Omar Baig, Dorika Steen, Juan J. Nogueira, *Molecules*, 2018, 23, 2932.

2 S. Mai, H. Gattuso, A. Monari and L. González, *Front. Chem.*, 2018, 6, 495.



3 E. R. Kjellgren, J. M. H. Olsen and J. Kongsted, *J. Chem. Theory Comput.*, 2018, 14, 4309–4319.

4 S. Valteau, A. Einfeld, A. Aspuru-guzik, S. Valteau, A. Einfeld and A. Aspuru-guzik, 2012, 137, 224103.

5 S. Mukamel, *Principles of nonlinear optical spectroscopy*, Oxford University Press, New York, 1995.

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## The Influence of Adsorption Geometry on Surface Catalytic Reactions

19 Jan  
10:30-10:50

Helen Eisenberg<sup>1,2</sup>, Iris Berg<sup>2</sup>, Shahar Dery<sup>2</sup>, Tehila Shahar<sup>2</sup>, Elad Gross<sup>2</sup> and Tamar Stein<sup>1,2</sup>

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The Hebrew University, Jerusalem 91904, Israel

Chemoselective reduction of nitro groups in nitroaromatics is a challenging catalytic process with high interest due to the importance of the resulting anilines for the chemical industry. Molecular-level understanding of the ways by which adsorption geometry of nitroaromatics influence their affinity toward nitro reduction will enable the development of highly selective catalysts. We performed experiments on para- and ortho-nitrothiophenol (NTP) self-assembled monolayers on Au (111) and Pt (111) catalytic surfaces, which showed that the reactivity of NTPs was directly influenced by their molecular conformation, and that surface proximity and orientation of the nitro group was a key parameter in its reduction. In order to further understand the molecular-level mechanisms behind the experimental results, we performed density functional theory (DFT) calculations to determine the adsorption geometry of these monolayers, their binding energy and to characterize the nitro-metal interaction. The binding energy of p-NTP increased with flatter orientation towards the horizontal metal surface. The nitro group in p-NTP was orientated in the plane of the molecule, and so bonding between the nitro group and the metal surface, and its reduction in experiments, was only observed when the nitro group was sufficiently close to the metal surface in the flatter orientations. For o-NTP the nitro group was orientated parallel, and in close proximity, to the surface, leading to bonding between the nitro group and the metal surface being observed for all o-NTP orientations, in agreement with the experimental observations of significant reduction of o-NTP at lower temperatures and in both flat and upright orientations. These results show that NTP nitro groups are only significantly reduced once they are positioned in high proximity and roughly parallel to the catalytic surface.

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19 Jan  
11:10-11:30

## Laser-cooling and trapping AlF molecules

Gerard Meijer

Fritz Haber Institute, Berlin, Germany

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19 Jan  
11:30-12:00

## Near accurate solutions to the many particle Schrödinger equation for systems with hundreds of atoms: opportunities and pitfalls

Frank Neese

Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany

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19 Jan  
12:45-13:05

## The exchange-correlation potential in density-functional theory: exact asymptotic behavior and strategy for advanced approximations

Eli Kraisler

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

Density functional theory (DFT) is nowadays the leading theoretical framework for quantum description of materials from first principles. The predictive power of DFT critically depends on an accurate approximation to the generally unknown exchange-correlation (xc) energy functional. Approximations to the xc functional can be and many times are constructed from first principles, by satisfying known properties of the exact functional. In this talk I focus on the behavior of the exact xc potential,  $v_{xc}(r)$ , and the exact xc energy-density-per-particle,  $\epsilon_{xc}(r)$  for very large  $r$  – far away from a finite, many-electron system. Several aspects of the behavior of the aforementioned quantities are presented. First, it is shown that the asymptotic form of  $v_{xc}(r)$  and  $\epsilon_{xc}(r)$  is independent: correct behavior of one does not guarantee the other. The relation between the two can be made via the xc hole response function, whose properties are discussed and its exact exchange part is analytically derived [1]. Furthermore, it is shown that the asymptotic behavior of  $v_{xc}(r)$  is not a direct consequence of the infamous self-interaction problem in DFT [2]. These are two separate issues to be addressed in the design of xc approximations. Second, the importance of reconstructing the sharp steps in the KS potential for an accurate prediction of the fundamental gap and the correct distribution of charge in complex systems is emphasized. The relationship between the derivative discontinuity and steps in stretched systems is exposed [3]. Third, the asymptotic behavior of the exact Pauli potential, an essential ingredient in orbital-free DFT, is presented [4]. Based on these findings, a strategy for development of advanced approximations for exchange and correlation with correct asymptotics is suggested.

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[2] T. Schmidt, E. Kraisler, L. Kronik and S. Kümmel, *Phys. Chem. Chem. Phys.* 16, 14357 (2014)

[3] M.J.P. Hodgson, E. Kraisler, A. Schild, E.K.U. Gross, *J. Phys. Chem. Lett.* 8 5974-5980 (2017)

[4] E. Kraisler, A. Schild, *Phys. Rev. Research* 2, 013159 (2020)

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## Smell loss and taste loss to predict COVID-19: Google searches and self-reports

19 Jan  
13:05-13:25

Kim Asseo and Masha Y. Niv

The Institute of Biochemistry, Food Science and Nutrition, The Faculty of Agriculture, Food and Environment, The Hebrew University of Jerusalem, Rehovot, Israel

Sudden onset of taste and smell loss have emerged as important symptoms of COVID-19. Several research and media (The New York Time, Washington Post and on CNBC) proposed that Google Trends searches on smell loss indicate or even predict new COVID-19 cases. Using US and Italy as test-cases, we have shown that correlation of the sensory symptoms with new COVID-19 cases for each country as a whole was high at some time points, but decreased (Italy) or dramatically fluctuated over time (US)<sup>1</sup>. Thus, simple tracking of popularity of taste and smell loss searches is not reliable for pandemic monitoring. On the other hand, in a case-controlled study of COVID-19 positive and COVID-19 negative patients in Israel, we have established that self-reported quantitative olfactory changes, by themselves or combined with other symptoms, provide a specific predictor of patient's COVID-19 status<sup>2</sup>. Our results suggest that ranking of the ability to smell before and during the illness, provides a practical approach with high predictive capability.

1. Asseo, K., Fierro, F., Slavutsky, Y., Frasnelli, J. and Niv, M. Y. Tracking COVID-19 using taste and smell loss Google searches is not a reliable strategy. *Sci. Rep.* 10, 20527 (2020).

2. Karni, N. et al. Self-rated smell ability enables highly specific predictors of COVID-19 status: a case control study in Israel. *medRxiv* 2020.07.30.20164327 (2020).

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19 Jan  
14:10-14:30

## Fermi Surface Reconstruction Without Symmetry Breaking

Snir Gazit

Racah Institute of Physics and The Fritz Haber Research Center for Molecular Dynamics, The Hebrew University of Jerusalem, Jerusalem 91904, Israel

I present a sign-problem-free quantum Monte Carlo study of a model that exhibits quantum phase transitions without symmetry breaking and associated changes in the size of the Fermi surface. The model is an Ising gauge theory on the square lattice coupled to an Ising matter field and spinful “orthogonal” fermions at half filling, both carrying Ising gauge charges. In contrast to previous studies, our model hosts an electronlike, gauge-neutral fermion excitation providing access to Fermi-liquid phases. One of the phases of the model is a previously studied orthogonal semimetal, which has  $\mathbb{Z}_2$  topological order and Luttinger-volume-violating Fermi points with gapless orthogonal fermion excitations. We elucidate the global phase diagram of the model: Along with a conventional Fermi-liquid phase with a large Luttinger-volume Fermi surface, we also find a “deconfined” Fermi liquid in which the large Fermi surface coexists with fractionalized excitations. We present results for the electron spectral function, showing its evolution from the orthogonal semimetal with a spectral weight near momenta  $\{\pi/2, \pi/2\}$  to a large Fermi surface.

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19 Jan  
14:30-14:50

## Ab-initio Forces from stochastic DFT: a formalism in a nonorthogonal basis-set representation

Ben Shpiro and Roi Baer

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

Stochastic density functional theory (sDFT) [1] is an ab-initio electronic structure method in which the scaling of the calculation with system size is reduced from cubic to linear and is thus applicable for treatment of mesoscopic systems. The reduced scaling is achieved as all expectation values are calculated as stochastic traces and therefore have statistical errors: a fluctuation and a bias. Noisy forces calculated from sDFT have been shown to be useful for geometry optimization when implemented in a Langevin dynamics framework [2] yet it is key to make sure the errors are governed by the fluctuations rather than the bias. A more recent development of sDFT, based on a joint grid and Gaussian basis set approach [3], allows for a more detailed analysis of the bias as well as applicability to larger systems. The use of a nonorthogonal basis requires additional challenges, most notably the calculation of the overlap inverse but also treatment of Pulay terms that are introduced in the forces acting on the nuclei. In this talk I will present a brand new formalism for the calculation of forces in a nonorthogonal basis-set representation. Results of stochastic forces calculations for the Tryptophan Zipper 2 peptide solvated in water and an analysis of the statistical errors under this new development showcase sDFT as a viable ab-initio method to calculate forces on biomolecules.

1. Baer R, Neuhauser D, Rabani E. Self-averaging stochastic Kohn-Sham density functional theory. *Phys Rev Lett.* 2013; 111:106402

2. Arnon E, Rabani E, Neuhauser D, Baer R. Efficient Langevin dynamics for "noisy" forces. *J Chem Phys.* 2020, 152, 161103.

3. Fabian MD\*, Shpiro B\*, Rabani E, Neuhauser D, Baer R. Stochastic density functional theory. *WIREs Comput Mol Sci.* 2019;e1412. \*Both authors contributed equally to this work

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## Unrestrained growth of correctly oriented microtubules is crucial for establishing axonal microtubule orientation

19 Jan  
14:50-15:10

Maximilian AH Jakobs<sup>1</sup>, Assaf Zemel<sup>2</sup>, Kristian Franze<sup>1,3</sup>

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<sup>2</sup>Institute of Dental Sciences and Fritz Haber Center for Molecular Dynamics, Hebrew University of Jerusalem, Jerusalem, Israel.

<sup>3</sup>Institute of Medical Physics, Friedrich-Alexander University Erlangen-Nuremberg, 91052 Erlangen, Germany.

Cellular transport of protein and genetic material requires oriented microtubules to guide vital nutrients to specific cellular compartments. Yet we do not know much about how microtubules self-orient. In neuronal axons, oriented microtubules are especially important since nutrients and genetic material have to be transported over vast distances. We here combined high throughput machine learning based imaging in *Drosophila melanogaster* axons with physical modeling and simulations and discovered that correctly oriented microtubules are more likely to exhibit persistent long-term growth than ill-oriented ones. We hypothesized that this enhanced growth is the root cause of microtubule orientation in axons. Accordingly, decreasing microtubule growth experimentally decreased the fraction of correctly oriented microtubules and computer simulations demonstrated that persistent growth of correctly oriented microtubules is essential to orient axonal microtubules

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## Vector potential in the exact factorization equations and its consequences for nuclear dynamics

19 Jan  
16:00-16:20

Ryan Requist, Eberhard K. U. Gross

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An effective vector potential analogous to the Mead-Truhlar molecular vector potential appears in the nuclear Schrödinger equation of the exact factorization method [1] – a theoretical framework for going beyond the Born-Oppenheimer approximation. Together with the potential energy surface, this vector potential fully mediates all electronic effects on the dynamics of a molecule. I will present two novel consequences of the vector potential.

First, it induces a Lorentz-type force in the equations of motion for the collective variables of the nuclear subsystem, namely the total momentum, angular momentum

and energy. We have derived generalized Ehrenfest identities that quantify the energy and momentum transfer between electrons and nuclei, and I will discuss how they can be applied in simulations of molecules and solids [2].

Second, the vector potential modifies the phonon modes of bulk crystals [3]. This is a general phenomenon in systems that break time-reversal symmetry and thus of great interest for magnetic materials. We have proposed a density functional-type approximation that opens up the possibility of performing calculations with an ab initio vector potential to investigate exciting emerging research topics such as the phonon Hall effect and spin-phonon-coupling effects.

[1] Abedi, Maitra, Gross, Phys. Rev. Lett. 105, 123002 (2010).

[2] Li, Requist, Gross, arxiv:1908.04077 (2019).

[3] Requist, Proetto, Gross, Phys. Rev. B. 99, 165136 (2019).

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## Surprisal of a quantum state: dynamics, compact representation and coherence effects

19 Jan  
16:20-16:40

K. Komarova, F. Remacle, and R.D. Levine

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

The state of a quantum mechanical system, pure or mixed, is described by a density operator. Surprisal – the logarithm of the density matrix – follows the same unitary evolution as the density operator. The maximal entropy formalism provides an explicit form of the density as an exponential function of a set of operators, whose observables are given. It allows to describe the state of the system explicitly via our knowledge about its observables [1-4]. The most well-known example of such a function is Boltzmann distribution,  $\hat{\rho} = \mathcal{Z}^{-1}e^{-\beta\hat{H}}$ , where the state of the system is defined by only one observable – energy. In general, there can be more than one operator that contributes to the density and these operators do not necessarily commute. Hence, the representation of the surprisal, logarithm of the exponential function, is a simpler construct than the density itself and allows more compact description of a quantum state. I will focus on a simple example of a non-adiabatic dynamics–non-radiative decay between two electronic states due to diabatic coupling, modeled after pyrazine [5]. In this example the electronic and nuclear degrees of freedom are coupled and coherence effects are prominent.

Ultrafast population exchange between two electronic states due to diabatic coupling

The wavepacket density on the upper electronic state is plotted in light green, and in dark grey on the lower electronic state as a function of normal mode nuclear coordinate,  $R$ . The panels are computed for increasing time values as indicated. Shown also are two approximate computations where the surprisal is expanded in a minimal basis of dominant constraints  $\{\hat{I}_N, \hat{a}, \hat{a}^\dagger, \hat{a}^\dagger\hat{a}\}$ , red dotted curve, and in an extended set  $\{\hat{I}_N, \hat{a}, \hat{a}^\dagger, \hat{a}^2, (\hat{a}^\dagger)^2, \hat{a}^\dagger\hat{a}\}$ , blue dashed curve.

[1] E. T. Jaynes, "Information Theory and Statistical Mechanics," Phys. Rev. 106, 620 (1957).

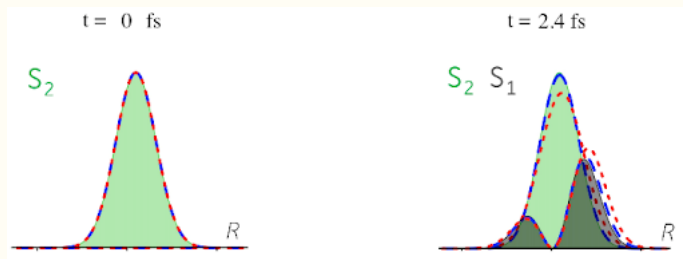


Figure 2: Ultrafast population exchange between two electronic states due to diabatic coupling

[2] E. H. Wichmann, "Density Matrices Arising from Incomplete Measurements," J. Math. Phys. 4, 884 (1963).

[3] R. D. Levine, "Information Theory Approach to Molecular Reaction Dynamics," Annu. Rev. Phys. Chem. 29, 59 (1978).

[4] Y. Alhassid and R. D. Levine, "Connection between the maximal entropy and the scattering theoretic analyses of collision processes," Phys. Rev. A 18, 89 (1978).

[5] R. Schneider, W. Domcke. S1-S2 Conical intersection and ultrafast S2  $\rightarrow$  S1 internal conversion in pyrazine. Chem. Phys. Lett. 150, 235 (1988).

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## The High Frequency Limit of Spectroscopy

Vladimir U. Nazarov<sup>1,2</sup>, Hadassah Elgavi-Sinai<sup>2</sup> and Roi Baer<sup>2</sup>

<sup>1</sup>Moscow Institute of Physics and Technology (National Research University)

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Hebrew University of Jerusalem

19 Jan  
17:15-17:35

We derive the high-frequency limit of optical spectroscopy, leading to a novel technique for imaging and characterizing a broad range of materials and compounds. Our theoretical development applies to any arbitrary atomic or molecular system within the clamped nuclei approximation, having dynamical and mutually interacting electrons. The system is exposed to the external time-dependent potential pulse,  $V(\mathbf{r}, t) = R(\mathbf{r})C(t) \cos(\omega_0 t)$ , where  $R(\mathbf{r})$  is the potential at spatial point  $\mathbf{r}$ ,  $C(t)$  is the enveloping function, i.e., the amplitude of the pulse at time  $t$ , and  $\omega_0$  is the pulse's frequency. At times  $t > T$ , where  $T$  is the pulse duration, and in the asymptotically large frequency  $\omega_0$  limit, we find that the leading term in the transition amplitude to a state  $|\alpha\rangle$  is proportional to  $\omega_0^{-n} C^2(E_\alpha - E_0)$ , where  $C^2(\omega)$  is the Fourier transform of the enveloping function squared  $C(t)^2$ , and  $E_\alpha$  are the eigenenergies. We further find that  $n = 2$  for all spatial forms of the potential  $R(\mathbf{r})$ , except for the important linear (dipole) case  $R(\mathbf{r}) = -\mathbf{E} \cdot \mathbf{r}$ , where the leading order is  $n = 4$ . Accordingly, upon the end of the pulse, the linear response is suppressed in the high carrier frequency limit, while, for the enveloping function  $C(t)$ , the quadratic response governs the excitation process. Application to the model systems of jellium slab and sphere reveals a richer excitation spectra than accessible in the linear-response regime, as well as high surface sensitivity of the proposed method. Despite



the essential nonlinearity of the considered regime, we show that observables can be conveniently expressed in terms of the linear density response function  $\chi(\mathbf{r}, \mathbf{r}', \omega)$ , allowing for the use of the efficient machinery of the linear response time-dependent density functional theory. Based on these findings, we propose a new spectroscopic technique. By combining the advantages of the extremely high surface sensitivity with probing the modes inaccessible or hardly accessible by other spectroscopies, the new technique is envisaged to evolve into a powerful characterization method in nanotechnology.

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### Dissociation in strong field: a quantum analysis of the relation between angular momentum and angular distribution of fragments

19 Jan  
17:35-17:55

Bar Ezra<sup>1</sup>, Shimshon Kallush<sup>1,2</sup>, Ronnie Kosloff<sup>1</sup>

<sup>1</sup>The Institute of Chemistry and the Fritz Haber Centre for Theoretical Chemistry, The Hebrew University of Jerusalem

<sup>2</sup>Department of Physics and Optical Engineering, ORT-Braude College

We studied the influence of field properties on the angular distribution of the outgoing fragments in the laboratory-fixed axis, defined by the field polarization. An ab initio model of strong-field photodissociation of diatomic molecules was developed. Simulating the full process is obstructed by a number of numerical complexities. For example, angular momentum algebra and the initial thermal state. As a result, the Hilbert space size increases tremendously with temperature. Final state analysis is performed after a carefully designed absorbing boundary condition. I will start with a brief introduction of the system and the model. Following, I will present the results for the two simpler transition dipole orientation. The results demonstrate that strong field leads to changes in angular distribution while the kinetic energy distribution is almost constant. At the end of the presentation, I will present recent results on a random phase approach and our further plans.

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### Catalytic transformations using small quantum systems: explicit protocols and applications to cooling

19 Jan  
17:55-18:15

Ivan Henao and Raam Uzdin

Fritz Haber Center for Molecular Dynamics Research, Institute of Chemistry, Hebrew University of Jerusalem, Israel.

Catalysis is a well known phenomenon in chemical sciences. It allows to assist chemical reactions by means of substances that keep themselves unaltered, known as catalysts. In quantum sciences, catalysis is also studied by modeling the catalyst as a quantum system whose initial and final states coincide. In this talk I will present recent results that we obtained about catalytic processes in quantum systems. We developed tools that allow to analyze a class of catalytic processes with broad interest in quantum thermodynamics and related areas. I will discuss



the application to cooling, which constitutes a paradigmatic thermodynamic task of fundamental and practical relevance. In this context, it is shown that catalysts allow to cool quantum systems below thresholds that otherwise cannot be surpassed. These catalytic processes are also distinguished by being explicit, which means that the state of the catalyst and the quantum evolution that implements the process are explicitly given. Thus, they complement the more abstract approach often adopted for quantum catalysis, and hopefully can contribute to understand the microscopic mechanisms of chemical catalysis.

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# Abstracts for Posters - Session I

## #1: Matsubara One-Body Green's Function Approach for Bond Breaking in Quantum Chemistry

19 Jan  
UNKNOWN

Rebecca Efrat Hadad and Roi Baer

Institute of Chemistry and The Fritz Haber Research Center, The Hebrew University of Jerusalem, Jerusalem, Israel

The electron structure theory together with Born-Oppenheimer approximation reduces the complexity of bond breaking, allows us to solve only for the electronic problem. Despite the developments achieved by these approximations, the electronic problem continues to be a computational challenge for large molecules due to the many-electron interactions which correlates them. The HF method provides an upper estimate to the total electronic energy with a typical accuracy of 0.5-1%. The missing negative energy is called “the correlation energy”, and is commonly divided into dynamical and non-dynamical contributions. The dynamical correlation is always exists and is the result of the movement of the electrons and the Coulomb repulsion between them. The non-dynamical correlation can appear when the excited states of the Hamiltonian are nearly degenerate with its ground state. Therefore the ground state wave function involves a limited number of significantly weighted determinants. The non-dynamical correlation is crucial for a proper description of bond breaking. We are investigating the performance of Matsubara Green's function (GF) theory in bond breaking. The Matsubara GF theory is an exact theory for determining an open electronic system's average energy in thermal equilibrium with a heat and electron reservoir at inverse temperature and chemical potential . Using the concept of self-energy introduced by Dyson, the Matsubara GF approach takes a form very similar to that of a single-reference electronic structure method. Despite this simple-looking form, when  $\beta \rightarrow \infty$ , the theory includes all the correlation effects, dynamical and non-dynamical implicitly, just as the FCI ground-state wave function does. This fact places the Matsubara GF theory unique in studying the most challenging computational challenges of electronic structure and quantum chemistry. These include the energy curves in configurations where chemical bonds are being ruptured or in systems that include open-shell radicals, transition metal atoms, etc. However, the Matsubara GF theory is impractical to implement exactly because its equation of motion depends on the two-body GF, which in turn depends on the three-body GF, etc. The traditional way to proceed is therefore through the concept of self-energy for which perturbation theory supplies approximations. We apply the GF2 approach that uses the second-order perturbation theory for the self-energy. Once this approximate self-energy is used, the

success of the resulting Matsubara GF approach is not guaranteed to be accurate. We show here the Matsubara Green's function method for bond breaking in H<sub>2</sub>, Li<sub>2</sub>, and BH molecules.

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## #2: Linking aqueous trehalose glass-to-liquid transition with hydrogen bonding properties

19 Jan  
12:00-12:45

Gil I. Olgenblum and Daniel Harries

Institute of Chemistry, the Fritz Haber Research Center, and the Harvey M. Kruger center for Nanoscience & Nanotechnology, The Hebrew University, Jerusalem 9190401, Israel

Molecular mixtures that form glassy materials play an important role in the survivability of many biological life forms, and hold important technological implications, from desiccation protection to cryopreservation. An important example is the disaccharide trehalose, which is known for its exceptional ability to thermodynamically stabilize biomacromolecules such as proteins, lipids, and DNA in the biologically active state. Of special interest is the transition from aqueous solution to the dense and highly concentrated glassy state of trehalose that has been implicated in bioadaptation of different organisms toward desiccation stress. The glassy state is a metastable form of a liquid that is known to form when trehalose-water mixtures are cooled below the melting temperature until at the glass transition temperature, the viscosity is large enough that relaxation is unattainable on experimental timescales. The link between the stabilization effect and the glassy state properties has not yet been resolved. A prominent property of glass-forming sugars is the complex hydrogen bonding network that constitutes both the sugar and water collectively. We use molecular dynamics simulations to decipher the link between the structure and properties of trehalose-water mixtures in both liquid and the supercooled glassy state. We have developed and employed a methodology that allows us to analyze the thermodynamics of hydrogen bonds in simulations at different water contents and temperatures.[1] Remarkably, this analysis is able to link the liquid to glass transition with changes in hydrogen bond characteristics as it is sensitive to the coupling of hydrogen bonded pairs to their surrounding upon transition. Because the link between hydrogen bonding and the glass transition is not evident in other conventional methods, we expect our findings to help resolve the properties of the glass and the mechanisms of its formation also in the presence of added macromolecules. [1] G. I. Olgenblum, L. Sapir, and D. Harries, "Properties of Aqueous Trehalose Mixtures: Glass Transition and Hydrogen Bonding," 2020.

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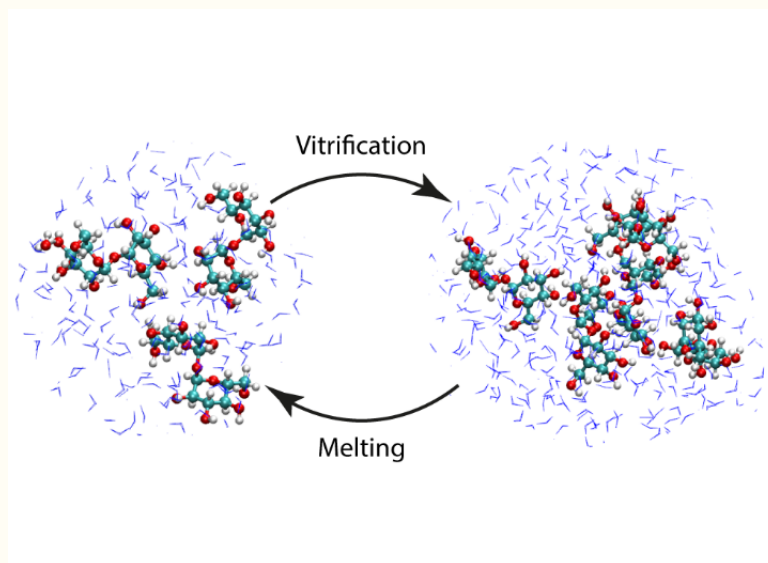


Figure 3:

### #3: Confinement in Nanodiscs Anisotropically Modifies Lipid Bilayer Elastic Properties

Itay Schachter, Christoph Allolio, George Khelashvili, and Daniel Harries.

The Fritz Haber Center, Institute of Chemistry, The Hebrew University of Jerusalem,  
Edmond J. Safra Campus, Givat Ram, Jerusalem 9190404, Israel.

19 Jan  
12:00-12:45

Lipid nanodiscs are small synthetic lipid bilayer structures that are stabilized in solution by special circumscribing (or scaffolding) proteins or polymers. Because they create native-like environments for transmembrane proteins, lipid nanodiscs have become a powerful tool for structural determination of this class of systems when combined with cryo-electron microscopy or nuclear magnetic resonance. The elastic properties of lipid bilayers determine how the lipid environment responds to membrane protein perturbations, and how the lipid in turn modifies the conformational state of the embedded protein. However, despite the abundant use of nanodiscs in determining membrane protein structure, the elastic material properties of even pure lipid nanodiscs (i.e., without embedded proteins) have not yet been quantitatively investigated before this work. A major hurdle is due to the inherently nonlocal treatment of the elastic properties of lipid systems implemented by most existing methods, both experimental and computational. Our group have previously described a computational analysis of molecular dynamics simulations designed to overcome these limitations, so it allows quantification of the bending rigidity ( $KC$ ) and tilt modulus ( $t$ ) on a local scale even for finite, nonperiodic systems, such as lipid nanodiscs. Here we use this computational approach to extract values of  $KC$  and  $t$  for a set of lipid nanodisc systems that vary in size and lipid composition. We find that the material properties of lipid nanodiscs are different from those of infinite bilayers of corresponding lipid composition, highlighting the effect of nanodisc confinement. Observed trends vary for nanodiscs of different size and composition.

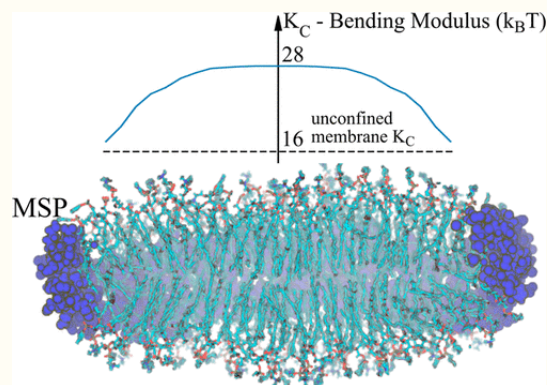


Figure 4:

## #4: A new density functional theory code for the exascale age

19 Jan  
12:00-12:45

Marcel Fabian

Fritz Haber Research Center of Molecular Dynamics, Institute of Chemistry, Edmond J. Safra Campus, The Hebrew University of Jerusalem, 9190401 Israel.

In the past few decades the massive computational power of supercomputers, has grown a million-fold and more. Within a few years exascale systems, affording at least one exaflops ( $10^{18}$  floating point operations per second) will become generally available. Exascale technology has the potential to revolutionize computational materials science, condensed matter physics, and quantum chemistry. However, for this to happen the massively parallel hardware must be accompanied by software and algorithms that can utilize the amount of processing power efficiently. Historically many quantum chemistry programs have struggled to parallelize beyond a few processors, due to large communication overhead and/or heavy I/O. We present here a new deterministic density functional theory (DFT) code that is highly parallelizable, is not I/O bound, scales linear in memory requirements with system size and exhibits linear weak scaling. Details of the algorithms are given as well as examples for the scaling behavior and validation of the code against Q-Chem.

## #5: Parallel Quantum Computation of Vibrational Dynamics

19 Jan  
12:00-12:45

Ksenia Komarova , Hugo Gattuso, R. D. Levine and F. Remacle

The Fritz Haber Center for Molecular Dynamics, Hebrew University of Jerusalem, Jerusalem, Israel.

Our quantum device is a solid-state array of semiconducting quantum dots that is addressed and read by 2D electronic spectroscopy [1, 2]. The experimental ultrafast dynamics of the device is well simulated by solving the time-dependent Schrödinger equation for a Hamiltonian that describes the lower electronically excited states of the dots and three laser pulses. The time evolution induced in the electronic states of the quantum device is used to emulate the quite different nonequilibrium vibrational

dynamics of a linear triatomic molecule. We simulate the energy transfer between the two local oscillators and, in a more elaborate application, the expectation values and variances of the quantum mechanical creation and annihilation operators of each local oscillator. The simulation uses the electronic coherences engineered in the device upon interaction with a specific sequence of ultrafast pulses. The algorithm uses the algebraic description of the dynamics of the physical problem and of the hardware. References 1. Parallel Quantum Computation of Vibrational Dynamics. K. Komarova, H. Gattuso, R.D. Levine, and F. Remacle. *Front. Phys.* 8, 590699, 2020.

2. Quantum Device Emulates Dynamics of Two Coupled Oscillators. K. Komarova, H. Gattuso, R.D. Levine, and F. Remacle. *J. Phys. Chem. Lett.* 11, 17, 6990–6995, 2020.

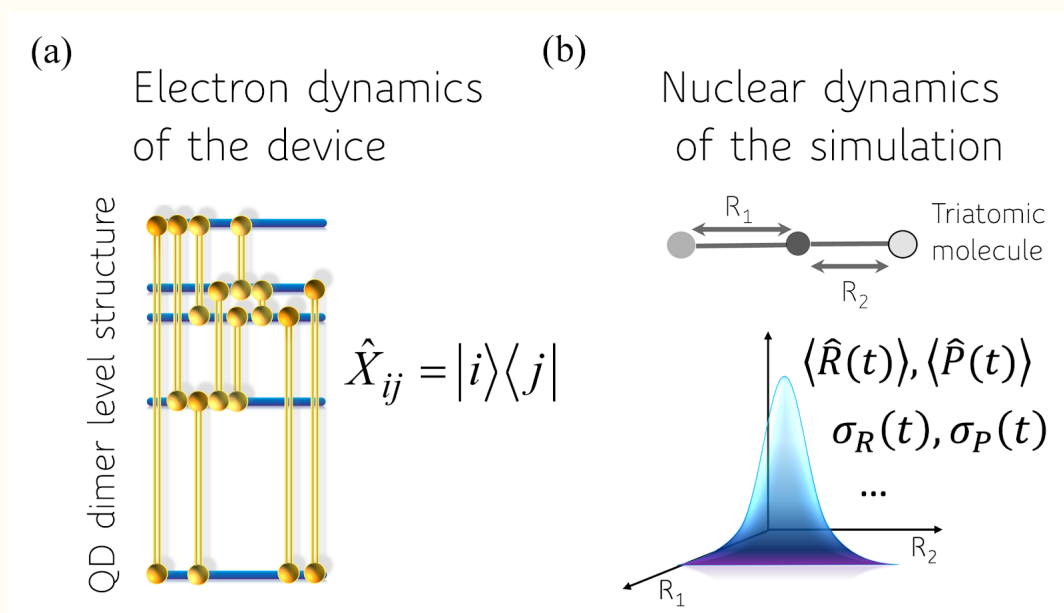


Figure 5: The four bands of excited electronic states of the device are indicated as well as the ten pairs  $i, j$  whose twenty corresponding coherences  $X_{ij}$  are used as logic variables.

## #6: Macroscopic polarization and topological invariants in strongly correlated systems

Ryan Requist and E. K. U. Gross

The Fritz Haber Center for Molecular Dynamics, Hebrew University of Jerusalem, Jerusalem, Israel.

19 Jan  
12:00-12:45

The macroscopic polarization of a solid is a fundamental quantity that determines ferroelectricity, piezoelectricity and other interesting properties. Topological invariants predict the presence of metallic states at the surface of an insulator. Both quantities are usually evaluated within mean-field band structure theory - an approach which is unreliable for strongly correlated systems. We present a simple

formula that approximates the macroscopic polarization in terms of the geometric phases of natural orbitals, the eigenfunctions of the one-body reduced density matrix. Numerical exact diagonalization of a strongly correlated one-dimensional model demonstrates that our formula accurately approximates the macroscopic polarization, even across the band insulator-Mott insulator transition. We show that natural orbitals can be used to estimate topological invariants in strongly correlated systems.

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## #7: Monte-Carlo study of a vertical stack of dipolar excitons

19 Jan  
12:00-12:45

Michal Zimmerman<sup>1</sup> S. Gazit<sup>1,2</sup>, R. Rapaport<sup>1</sup>

<sup>1</sup> The Racah Institute of Physics, The Hebrew University of Jerusalem, Jerusalem 9190401, Israel <sup>2</sup> The Fritz Haber Research Center for Molecular Dynamics, The Hebrew University of Jerusalem, Jerusalem 9190401, Israel

The long-range and anisotropic nature of dipolar interactions can stabilize many exotic phases, including supersolidity, spin-liquids, and unconventional superfluidity. Currently, dipolar fluids are studied primarily in cold atomic gases, where recent experiments have exemplified a supersolid phase [1-3]. A recent work by our group [4] presents the first observation of attractive dipolar interactions between coupled dipolar exciton fluids trapped in adjacent semiconductor bilayers. It was shown that the spatial distribution of the exciton fluids is modified due to attractive inter-layer interactions. Also, an increase of up to 7 meV in the binding energy was observed compared to the one expected due to two-body interactions. Here we present first results for the inter- and intra- layer density correlation functions obtained by numerical quantum Monte-Carlo simulations. The experimental system is modeled as dipolar bosons confined in a 2d bilayer structure with a fixed vertical separation. Extending the work of [5], we study the influence of imbalance in the densities of the layers, accounting for the density-dependent experimental measurements. Starting from balanced densities tuned to a paired superfluid phase, our numerical results indicate that density imbalance strongly affects the inter-layer and intra-layer correlation functions. In particular, we find that correlation peaks associated with the interparticle separation are smeared, compared to the balanced case [5]. This phenomenon is attributed to attractive inter-layer interactions, which, if sufficiently strong, give rise to a loss of extended range spatial order. Our simulation provides a powerful tool to numerically study many-body phases with strong anisotropic interactions and sheds light on the ongoing experimental efforts in this field. References [1] L. Chomaz, D. Petter, P. Ilzhöfer, G. Natale, A. Trautmann, C. Politi, G. Durastante, R.M.W. van Bijnen, A. Patscheider, M. Sohmen, M.J. Mark, and F. Ferlaino, Long-Lived and Transient Supersolid Behaviors in Dipolar Quantum Gases, *Phys. Rev. X* 9, 021012 (2019).

[2] L. Tanzi, E. Lucioni, F. Fama, J. Catani, A. Fioretti, C. Gabbanini, R. N. Bisset, L. Santos, and G. Modugno, Observation of a Dipolar Quantum Gas with Metastable Supersolid Properties, *Phys. Rev. Lett.* 122, 130405 (2019).



[3] F. Böttcher, J.-N. Schmidt, M. Wenzel, J. Hertkorn, M. Guo, T. Langen, and T. Pfau, Transient Supersolid Properties in an Array of Dipolar Quantum Droplets, *Phys. Rev. X* 9, 011051 (2019).

[4] C. Hubert, Y. Baruchi, Y. Harpaz, K. Cohen, K. Biermann, M. Lemeshko, K. West, L. N. Pfeiffer, R. Rapaport and P. V. Santos, Attractive Dipolar Coupling between Stacked Exciton Fluids, *Phys. Rev. X* 9, 021026 (2019).

[5] F. Cinti, D.W. Wang, M. Boninsegni, Phases of dipolar bosons in a bilayer geometry, *Phys. Rev. A* 95, 023622 (2017).

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## #8: Photochemistry of Insecticides: Theory and Experiment

19 Jan  
12:00-12:45

Dorit Shemesh, Barbara J. Finlayson-Pitts and R. Benny Gerber

The Fritz Haber Research Center and Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel

Neonicotinoid insecticides, which represents on third of the total insecticide market, are widely used to control sucking insect pest. As a result they are found on a variety of surfaces in the environment. They are generally believed to have low toxicity to non-target species. However, once in the environment, insecticides undergo photochemical and thermal reactions that lead to the formation of products whose toxicity can differ from that of the parent compound. In this poster we present quantum chemical calculations combined with experiments that explore photochemical reactions and photoabsorption spectra of two insecticides, namely imidacloprid and nitenpyram.

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## #9: Structures, Stability and Decomposition of the building blocks of the polynitrogen ionic solid $N_5^+B(N_3)_4^-$

19 Jan  
12:00-12:45

Itai Zakai R. Benny Gerber

The Fritz Haber Research Center and Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel

Polynitrogen materials are predicted to be highly energetic and are also interesting for their unknown properties and chemistry. The ionic solid  $N_5^+B(N_3)_4^-$  was prepared in the laboratory of Prof. Karl O. Christe in 2004, and it is one of the very few polynitrogens to be synthesized to date. In this work, we studied the structures and decomposition dynamics of the building blocks of this solid, the  $N_5^+B(N_3)_4^-$  monomer and the  $[N_5^+]_2[B(N_3)_4^-]_2$  dimer, by computer simulations that employ ab initio potentials.

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# Abstracts for Posters - Session II

## #1: Involvement of triplet state in isomerization of retinal analogs

19 Jan  
15:10-16:00

Ofer Filiba , Igor Schapiro The Fritz Haber Research Center and Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel

In this work we studied the involvement of a triplet state in the photoisomerization of the retinal protonated Schiff-base (RPSB) and its analogs. This is the initial process in the photocycle of the rhodopsin. Here we use quantum chemical calculations to understand this light-induced reaction with focus on the involvement of the triplet state. Three molecules were studied: protonated Schiff base (PSB), Schiff base (i.e. deprotonated SB), and aldehydes (ALDE). For each molecule three models were investigated with three, four and five double bonds. All calculations in this work were performed at the extended multi-state complete active space second order perturbation (XMS-CASPT2) level of theory using cc-pVDZ basis set. The XMS-CASPT2 method is employed to obtain the optimized ground state geometry, the minimum energy conical intersection (MECI) and the excitation energies along the unrelaxed scan. To estimate the reactivity in the excited state, we have interpolated geometries between the Franck-Condon point and the MECI. We have found that: (1) the MECI(S0,S1) of the PSB models shift to higher energies when increasing the number of double bonds, while for the SB models this trend is inverted; (2) the MECI(S0,S1) of the ALDE models remains relatively unchanged with respect to the number of double bonds; (3) according to El-Sayed rule, the intersystem crossing is possible after reaching the MECI(S1,S2) and before or at the MECI(S0,S1) of ALDE3/4 and SB3 models; (4) the involvement of the triplet state in the photochemistry of PSB is negligible, while for SB and ALDE is more probable.

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## #2: Structure-based screening for discovery of sweet compounds

19 Jan  
15:10-16:00

Yaron Ben Shoshan-Galeczki<sup>1</sup> , Christian Schmid<sup>2</sup> , Corinna Dawid<sup>2</sup>, Thomas Hofmann<sup>2</sup> and Masha Y Niv<sup>1</sup>

<sup>1</sup> The Institute of Biochemistry, Food and Nutrition, The Robert H Smith Faculty of Agriculture, Food and Environment, The Hebrew University, 76100 Rehovot and The Fritz Haber Center for Molecular Dynamics, The Hebrew University, Jerusalem, 91904, Israel. <sup>2</sup> Chair of Food Chemistry and Molecular Sensory Science, Technical University of Munich, Lise-Meitner-Str. 34, 85354 Freising, Germany

Sweet taste is a cue for calorie-rich food and is innately attractive to animals, including humans. In the context of modern diets, attraction to sweetness presents a significant challenge to human health. Most known sugars and sweeteners bind to the Venus Fly Trap domain of T1R2 subunit of the sweet taste heterodimer. Since the sweet taste receptor structure has not yet been experimentally solved, a possible approach to finding sweet molecules is virtual screening using compatibility of candidate molecules to homology models of sugar-binding site [1]. Here, the constructed structural models, docking and scoring schemes were validated by their ability to rank known sweet tasting compounds higher than properties-matched random molecules. The best performing models were next used in virtual screening, retrieving recently patented sweeteners and providing novel predictions. Next, the model was used for rationalizing structure-activity relationship of compounds derived from licorice, and to discriminate sweet from non-sweet compounds [2].

[1] Yaron Ben Shoshan-Galeczki and Masha Y. Niv ” Structure-based screening for discovery of sweet compounds”, Food Chemistry (2020).

[2] Christian Schmid, Corinna Dawid, Yaron Ben Shoshan-Galeczki, Anne Brockhoff, Timo Stark, Rukiye Erkaya, Maximilian Kranz, Masha Y. Niv, Wolfgang Meyerhof, and Thomas Hofmann, in preparation (2020).

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19 Jan  
15:10-16:00

### #3: Oxocarbenium Ion Conformer Dynamics

Michelle Dvores and R. Benny Gerber

The Fritz Haber Research Center and Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel

The oxocarbenium ion is thought to be the key intermediate in reactions of sugars. Recent gas phase spectroscopy experiments have provided the structures of these very transient intermediates. Here, in collaboration with gas phase IRMPD spectra experiments of John Simons, Pierre Çarçabal and Philippe Maître, we describe oxocarbenium ion conformer transitions from molecular dynamics simulations of protonated sugar species. Findings include distinct patterns of conformer transitions for oxocarbenium ion epimers and a surprising equivalence of structures between a sugar’s oxocarbenium ion and its anhydrosugar on the femtosecond timescale.

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#### #4: BitterMatch: prediction of ligand-receptor association inspired by Netflix

19 Jan  
15:10-16:00

Eitan Margulis Eitan Margulis, Yuli Slavutsky, Yuval Benjamini, Masha Y. Niv

The Institute of Biochemistry, Food and Nutrition, The Robert H Smith Faculty of Agriculture, Food and Environment, The Hebrew University, 76100 Rehovot and The Fritz Haber Center for Molecular Dynamics, The Hebrew University, Jerusalem, 91904, Israel.

Bitter taste receptors (T2Rs), are a subfamily of class A GPCRs,<sup>1</sup> capable of recognizing over 1000 chemically diverse ligands.<sup>2</sup> While some T2Rs are broadly tuned with more than 100 ligands, others are very selective with very few known ligands.<sup>3</sup> We present BitterMatch, a novel algorithm that is capable of matching ligands with their putative human and mouse T2Rs. The algorithm uses chemical and structural features of the ligands and the receptors. In addition, it uses the already known ligand-receptor (“customer-product”) associations, similarly to recommendation systems used in Netflix, YouTube and more. BitterMatch performance is currently estimated at AUC of 0.984 compared to random assignment, with precision of 80% and recall of 48%. Analysis of the contributing features revealed that the recommendation part of the algorithm is contributing to the prediction, together with structural features of the binding site and ligand properties. BitterMatch enables the discovery of new ligands for T2Rs as well as for other receptors with shared ligands. Potentially, BitterMatch could shed light on possible evolutionary roles of T2Rs, connections between T2Rs and other GPCRs and more.

References 1. Di Pizio, A. et al. Comparing Class A GPCRs to bitter taste receptors: Structural motifs, ligand interactions and agonist-to-antagonist ratios. *Methods Cell Biol.* 132, 401–427 (2016). 2. Dagan-Wiener, A. et al. BitterDB: taste ligands and receptors database in 2019. *Nucleic Acids Res.* 1–7 (2018). doi:10.1093/nar/gky974 3. Di Pizio, A. Niv, M. Y. Promiscuity and selectivity of bitter molecules and their receptors. *Bioorganic Med. Chem.* 23, 4082–4091 (2015).

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#### #5: Spectral Tuning Study in the Bistable Jumping Spider Rhodopsin-1: The Impact of Retinal Conformation.

19 Jan  
15:10-16:00

Jonathan R. Church and Igor Schapiro

Fritz Haber Center for Molecular Dynamics Research, Institute of Chemistry, Hebrew University of Jerusalem, Israel.

Jumping Spider Rhodopsin-1 (JSR1) is a bistable retinal protein. In bistable rhodopsins both the dark state and photoproduct are thermally stable and can be interconverted through absorption of a photon. In this work hybrid QM/MM simulations were performed to study the 9-cis, 11-cis and all-trans conformations of retinal based on a recently published crystal structure of JRS1. Because only the 9-cis crystal structure is available, the 11-cis and all-trans chromophores were modelled using Squid Rhodopsin structures due to their similarity. The absorption shifts between the various forms of the chromophore were then calculated and analyzed. This was done

by producing thermally sampled snapshots using a QM/MM trajectory and analyzing excitation energies using RI-ADC(2) and TD-DFT. To observe the impact the environment plays in the absorption shifts comparison spectra were produced by removing the protein environment. Additionally, the electrostatic potential of the environment was projected onto each retinal chromophore using a point charge model to visualize any stabilizing effects produced by the protein.

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## #6: Photoconversion of Phycocyanobilin in the red/green Cyanobacteriochrome AnPixJg2

19 Jan  
15:10-16:00

Aditya Rao and Igor Schapiro

Fritz Haber Center for Molecular Dynamics Research, Institute of Chemistry, Hebrew University of Jerusalem, Israel.

Cyanobacteriochromes (CBCRs) are recently discovered members of the phytochrome superfamily 1. Like phytochromes they bind a linear tetrapyrrole as a chromophore but in contrast, CBCRs require only the GAF domain for their function. There are at least four different sub-families known in CBCRs out of which the red/green CBCRs have a red-absorbing reactant and a green-absorbing photoproduct. Upon light illumination, the PCB chromophore in the red/green CBCR AnPixJg2 undergoes a reversible photoisomerization around the C15=C16 double bond <sup>2</sup> with a concomitant rotation of the D-ring. To elucidate the mechanism of the isomerization of PCB, we have carried out excited state relaxed scans of minimal models within gas-phase using time-dependent density functional theory (TD-DFT) and second order algebraic diagrammatic construction scheme (ADC(2)) <sup>3</sup>. Also, to probe the effect of the protein environment, we have carried out relaxed scans including the protein using the hybrid QM/MM methodology.

(1) Rockwell, N. C.; Ohlendorf, R.; Möglich, A. Proc. Natl. Acad. Sci. USA 2013, 110 (3), 806–807.

(2) Narikawa, R.; Fukushima, Y.; Ishizuka, T.; Itoh, S.; Ikeuchi, M. J. Mol. Biol. 2008, 380 (5), 844–855.

(3) Schirmer, J. Phys. Rev. A 1982, 26 (5), 2395–2416.

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## #7: Thermodynamic-based bounds on periodically driven quantum systems

19 Jan  
15:10-16:00

Tanmoy Pandit and Raam Uzdin

The Fritz Haber Research Center and Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel

Traditionally in quantum and/or non-Markovian thermodynamics second-law-like bounds deal with two time points: the initial and the final. For periodically driven systems we find a set of thermodynamics bounds that deal with midpoints of the evolution. For pure initial states, the observable being constrained to the survival probability. We use these bounds to detect leakage due to unaccounted environments in quantum circuits as well as for detecting deviation from perfect periodic driving. We demonstrated experimentally our findings in IBM quantum processor. Specifically, we provide two experimental examples where these bounds outperform fundamental bounds on leakage detection based on the previously used 1 cycle detection scheme (including the second law of thermodynamics). The derived bounds treat the driven circuits as a blackbox and makes no assumptions on it.

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## #8: How Urea Counteracts Trimethylamine N-oxide Induced Attraction Between Lipid Membranes

19 Jan  
15:10-16:00

Yuri Shakhman<sup>1</sup>, Shahar Sukenik<sup>2</sup> and Daniel Harries<sup>1</sup>

<sup>1</sup> The Fritz Haber Research Center and Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel

<sup>2</sup> Chemistry and Chemical Biology, UC Merced, Merced, CA, USA

Elasmobranchii such as sharks, accumulate small organic molecules called osmolytes in concentrations at the molar range, as an osmoregulatory strategy to counteract the detrimental effects of the surrounding seawater on cells and their constituents. Curiously, two osmolytes, TMAO and urea, act together in sharks to form solutions at molar concentrations whose net action is close to that of pure water. Although it is known that many osmolytes exert an apparent attractive or repulsive force between self-assembled lipid membranes, all proposed models fail to fully account for the origin of this force. Toward resolving the mechanism by which osmolytes modulate lipid interactions, we followed several osmolytes, including urea and TMAO and their interactions with lipid membranes in aqueous solution. We found that TMAO pushes adjacent membranes closer together, while urea makes membranes grow further apart. Experiments and simulations further show that the change in the force between membranes is due to the partitioning of TMAO away from the volume between bilayers. This in turn stems from the exclusion of TMAO from the lipid-water interface. Hence the underlying mechanism resembles protein stabilization by osmolytes. By contrast urea is equally partitioned in lipid and bulk, and its action is related to modified van der Waals interactions. Interestingly, urea and TMAO act synergistically, so that the presence of one changes the preferential interaction of the other with lipids. We discuss the potential role of osmolytes acting together in the modification of membrane remodeling events.

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## #9: Solving the Lindbladian Problem with the help of Stochastic Schrodinger Equation

19 Jan  
15:10-16:00

Sayak Adhikari and Roi Baer

Fritz Haber Research Center of Molecular Dynamics, Institute of Chemistry, Edmond J. Safra Campus, The Hebrew University of Jerusalem, 9190401 Israel.

The Lindblad equation is usually used to study the dynamics of an open quantum system. This is very much of importance to other varieties of fields, such as atomic physics, materials science, quantum biology. For canonical systems, the Lindbladian dynamics becomes complicated for electrons even when mutual Coulomb repulsion is omitted as one of the constraints. This happens because they are still able to affect each other by interacting with the bath. Here, we develop an approach, based on the Ito-Taylor expansion, which allows us to evolve non-interacting electrons in open quantum systems. We evolve a system by using commutative operators in the Stochastic Schrodinger equation so we have analytical answers by diagonalizing the equations and check the strong and weak convergence behaviour of the Ito-Taylor expansion equations. Then we modified the equations further to incorporate complex Wiener Processes. Furthermore we started to use non-commutative operators and started to check the weak convergence behaviour with the analytical answers we obtain from the Lindblad master equation. Here, after evolving the wavefunction we compared the density matrix of the evolved system and the density matrix we solve from the Lindblad equation. We are now using our modified Ito-Taylor expansions to check on larger systems and then we will use it on systems of trapped electrons.

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## #10: Discovery of agonists and antagonists targeting bitter taste receptor homology models.

19 Jan  
15:10-16:00

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Since when bitter taste receptors (T2Rs) have been identified in the taste buds of the tongue as the proteins responsible for bitter compounds detection, our knowledge on this GPCRs subfamily widely increased. Indeed, extraoral T2Rs have been identified, associated with several physiological/pathological processes. Therefore, discovery of ligands targeting and modulating T2Rs activity (agonist and antagonist) can help in food research, as well as in pharmacological applications. Molecular insight into T2Rs ligand binding is obstructed by the lack of experimental 3D structures. Furthermore, the low sequence identity ( 15%) with available GPCR templates results in low resolution homology models. An accurate combination of computational methods (homology modelling, docking, virtual screening) with experimental data has already shown to be able to overcome these

limitations [1]. Here, we focused our attention on bitter taste receptor TAS2R14, involved in extraoral roles like mucociliary clearance in the sinonasal cilia and muscular contraction in the heart myocytes. In order to find new compounds targeting



T2R14, we set up a methodology that allow us to increase the homology models reliability. Upon generation of the model, induced fit docking or normal mode analysis were used to increase the conformational space exploration of the receptor binding site. Evaluation of these receptor model's ability to discriminate between active compounds and a list of decoys has been performed using docking followed by calculation of enrichment factors and ROC-AUC. The two homology models showing best performances in agonists or antagonists identification were selected and used to successfully suggest new drugs through virtual screening of a large library of compounds. References: 1.) Di Pizio A, Waterloo LAW, Brox R, Löber S, Weikert D, Behrens M, Gmeiner P Niv MY, Cellular and Molecular Life Sciences, 2020, 77, 531-542.



Figure 6:

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