Poster Session Industry

Poster Session II: BIOLOGICAL PHYSICS (DBIO)

11:30 am – 2:30 pm, Wednesday March 19 // Session MAR-M00 (DBIO) //
Anaheim Convention Center, Exhibit Hall A

Chair: Elizabeth Udeh, University of Kansas

Topics: AI/Machine Learning; Active Matter; Animal Behavior; Applications; Bio-Inspired Phase Separation … Show all topics

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Self-Consistent Method for Studying Excitation Energy Transfer in Multichromophoric Systems

Poster 252

Presenter: Veljko Jankovic (Institute of Physics Belgrade, University of Belgrade)

Author: Tomáš Mančal (Faculty of Mathematics and Physics, Charles University, Prague)

Further progress in fundamental understanding of the initial steps of solar-energy conversion in both natural and artificial systems requires computationally inexpensive yet reasonably accurate methods for excited-state quantum dynamics.

Starting from the memory kernel in Born approximation, and recognizing the quantum master equation as the Dyson equation of the Green's functions theory, we formulate the self-consistent Born approximation (SCBA) to resum the memory-kernel perturbation series in powers of the exciton–environment interaction [1]. Our SCBA is formulated in the Liouville space and frequency domain, and it handles arbitrary spectral densities of the interaction.

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Membrane potential mediates the cellular response to mechanical pressure
Markus Basan (presenter)

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Antimicrobial Peptides as Broad-Spectrum Therapeutics: Machine Learning-Based Modelling of Multi-Target Activity
Anatoly B Kolomeisky (presenter), Catherine Vasnetsov, Victor Vasnetsov

Poster 221
Revealing EPS1's Catalytic Mechanism in the Biosynthesis of Salicylic Acid via Computer Modeling
Tianjie Li (presenter), Yi Wang

Poster 222
Deciphering the role of phosphorylation in tau fibril formation using genetic code expansion
Edward Lien (presenter), Cat Hoang Vesely, Ryan Higa, Richard B Cooley, Peter J Chung

In a molecular dimer coupled to an overdamped oscillator environment, we find that the SCBA reproduces the true exciton dynamics very well even in the most challenging regimes of strong interactions, slow environments, and low temperatures. While the SCBA is good (poor) at describing energy transfer modulated by an underdamped vibration resonant (off-resonant) with the exciton energy gap, we find it reasonably describes exciton dynamics in the seven-site model of the Fenna–Matthews–Olson complex in a realistic environment comprising both an overdamped continuum and underdamped vibrations.

Poster 223

Targeting Tumors: How Lipids and Ions Influence pHLIP Membrane Partitioning

Thi Huong Quynh Nguyen (presenter), Douglas J Tobias, Alexey Ladokhin

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