

Physical Chemistry Seminar

Towards ab initio simulations of driven and non-equilibrium systems through novel theoretical and numerical approaches

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In this talk, I will discuss the recent developments in the many-body perturbation theory in Green's function formulation, aiming to capture the (driven) dynamical correlations in realistic nanoscale condensed matter systems. Compared to the equilibrium methods, the out-of-equilibrium phenomena suffer from additional computational and theoretical bottlenecks manifested through the time non-local terms, leading to prohibitively costly simulations using the common condensed matter electronic structure approaches. I will, in particular, focus on overcoming these hurdles in non-equilibrium dynamics calculations and the possible truncations and reformulations of time-nonlocal quantum interactions. I will present numerical and data-driven methods, as well as a novel real-time Dyson expansion formalism that captures the non-equilibrium physics of driven systems exhibiting emergent quasiparticle phenomena. Among other advantages, it can be readily deployed together with real-time random sampling approaches, which revolutionized the calculations employing Green's function formalism and allow simulations of systems with tens of thousands of electrons at GW and post-GW levels.



Wednesday, November 6, 2024



10:30am



BRWN 4102



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Vlcek Bio

Dr. Vlcek received his PhD in 2016 jointly from The Hebrew University of Jerusalem (Israel) and the University of Bayreuth (Germany), where he studied in the chemistry and physics departments. His PhD was sponsored by the Minerva Fellowship of the Max Planck Society. From 2016 to 2018, Dr. Vlcek continued as a postdoctoral researcher at UCLA in the Department of Chemistry and Biochemistry. He joined the faculty at UCSB in 2018. In 2020, he received the NSF Career Award; he was selected as an Emerging Investigator by the Journal of Chemical Physics (2019) and as an Emerging Leader by the Journal of Physics Condensed Matter (2020). In 2024, he received the Sloan Research Fellowship.