DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE
SEMINAR SERIES
SPRING 2019

DATE: TUESDAY, APRIL 9
LOCATION: Central King Bldg. - 303
TIME: 1:00pm – 2:20pm

GUEST SPEAKER

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TOPIC

Open Quantum Subsystem Dynamics in Liquids and Molecules at Surfaces

ABSTRACT

Leveraging an open-subsystem formulation of Density Functional Theory (DFT) [1] we aim at describing periodic and molecular systems alike, including their electronic and nuclear dynamics. Subsystem DFT enables first principles simulations to approach realistic time- and length-scales, and most importantly sheds light on the dynamical behavior of complex systems. Taking subsystem DFT to the time domain allows us to inspect the electron dynamics of condensed-phase systems in real time. In liquids and interfaces, we observe all the relevant regimes proper of non-Markovian open quantum system dynamics, such as electronic energy transfer, and screening [2]. In addition, the ab-initio modeling of system-bath interactions brought us to observe and justify the holographic time-dependent electron density theorem. Contrary to interactions between molecular (finite) systems, when molecules interact with metal or semiconductor surfaces [3] the electron dynamics is strongly non-Markovian with dramatic repercussions to the molecule's response to external perturbations. Metals and semiconductors typically have large polarizabilities, and even in a regime of low coupling their effect on impinging molecular species is significant – line broadening, peak shift, and intensity borrowing are observed, characterized, and explained in terms of inter-subsystem dynamical interactions and a many-body decomposition of the system's density-density response function in a way that transcends the canons of Fermi Golden Rule.

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References

[1] Michele Pavanello, *The Journal of Chemical Physics* 138 (2013) 204118.
[2] Sudheer Kumar P., Alessandro Genova and Michele Pavanello *The Journal of Physical Chemistry Letters* 8 (2017) 5077-5083.
[3] Alina Umerbekova, Shou-Feng Zhang, Sudheer Kumar P., and Michele Pavanello, *The European Physical Journal B* 91 (2018) 214.

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