SPRING 2021 CHEMISTRY SEMINAR SERIES

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HOST:
DR. PAVANELLO
JOINT WITH PHYSICS

ALL THOSE INTERESTED ARE WELCOME TO ATTEND

Harnessing Model Kernels in Linear-Response Time-Dependent Density Functional Theory

March 5th, 2021 ~ 11:30AM

Seminar Via Zoom

Abstract: Time-dependent density functional (TDDFT) is an extension of density functional theory to time-dependent potentials. TDDFT is a computationally more feasible approximation to compute excitation energies, compared to approaches based on many-body techniques. The accuracy of TDDFT is restricted by the limitations of the exchange-correlation kernels that are commonly in use. Dynamical contributions can be improved when frequency-dependence is included, but in addition to frequency-dependence a sophisticated spatial nonlocality of the kernel is also required. In this work a dynamic model exchange-correlation kernel, the MCP07 based on exact constraints is introduced [1]. For the static limit, we modified the model of Constantin and Pitarke [2] at small wavevector q to recover the known second-order gradient expansion, plus other changes. For the zero-wavevector limit, we use the frequency-dependent Gross-Kohn kernel [3,4]. The dynamic MCP07 exchange-correlation kernel predicts a static charge-density wave at low densities and delivers excellent quality correlation energies for the ground state, while it predicts a plausible finite plasmon lifetime at all wavevectors for the first time within TDDFT.

The attractive features of the dynamic MCP07 kernel can be further exploited for gaining more insight about strong correlation [5]. Strong correlations within a symmetry-unbroken ground-state wavefunction can show up in approximate density functional theory as symmetry-broken spin-densities or total densities. They can arise from soft modes of fluctuations (sometimes collective excitations) such as spin-density or charge density waves at non-zero wavevector. Familiar examples are the unobservable but revealing symmetry breaking in stretched H2 and the observable symmetry breaking in antiferromagnetic solids. The example discussed here is the static charge-density wave/Wigner crystal phase of a low density (69) jellium. TDDFT is used to show quantitatively that the static charge density wave is a soft plasmon.

The MCP07 kernel has a potential impact on optical spectroscopy. Work along this direction will be also briefly discussed.

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[2] L.A. Constantin and J.M. Pitarke, Phys. Rev. B **78**, 245127 (2007)
[3] E.K.U. Gross and W. Kohn, Phys. Rev. Lett. **55**, 2850 (1985). Erratum *ibid.* **57**, 923 (1986)
[4] N. Iwamoto and E.K.U. Gross, Phys. Rev. B **35**, 3003 (1987)
[5] J. P. Perdew, A. Ruzsinszky, J. Sun, N. K. Nepal, and A. D. Kaplan, to appear in Proceedings of the National Academy of Sciences of the United States of America.

Biography: Adrienn Ruzsinszky received her Ph.D. from the University of Technology and Economics in Budapest in 2004. In 2003 she was awarded by the Pro Progressio Award for her work as a PhD student. After obtaining the PhD degree she moved to the USA and continued her work as a postdoc at Tulane University. In 2011 she joined the faculty at Tulane University as Research Assistant Professor of Physics. In 2013 she moved to the College of Science and Technology at Temple University as an Assistant Professor of Physics. Currently she is Associate Professor at the same place. Professor Ruzsinszky's research area includes Linear Response Time Dependent Density Functional Theory, development and applications of Density Functional Theory and Computational Materials Science. She is the recipient of the NSF CAREER award and the Humboldt Fellowship for experienced researchers.

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