Physics AT QUEENS COLLEGE

Colloquium Notice

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First-principle approach to strongly coupled light-matter systems

In recent years, research at the interface of material science, chemistry, and quantum optics has surged and now offers new possibilities to study light-matter interactions. The combination of theoretical concepts from these fields presents an opportunity to create a predictive theoretical and computational approach from first principles that describes the correlated dynamics of electrons, nuclei, and the electromagnetic field on the same quantized footing.
In this talk, we discuss how density-functional theory can be generalized to quantum-electrodynamical density-functional theory (QEDFT) and introduce electron-photon exchange-correlation functionals. The presented approach, photon MBD (pMBD), is inspired by the many-body dispersion (MBD) method for weak intermolecular interactions, which is generalized to include both electronic and photonic (electromagnetic) degrees of freedom on the same footing. We demonstrate that pMBD accurately captures effects that arise in the context of strong light-matter interactions, such as anisotropic electron-photon interactions, beyond single-photon effects, and cavity modulated van der Waals interactions. Moreover, we show that pMBD is computationally efficient and allows simulations of large complex systems coupled to optical cavities.

Monday
October 19, 2026
Starts at 12:15 PM
Coffee at 12:00 PM
Physics Conference Room, SB B326
This talk is accessible via **Zoom** or use
meeting ID 829 2687 2594 and **passcode 866995** to join