Title: London Dispersion, Density-Functional Theory, and Molecular Crystals

Abstract:
Inclusion of London dispersion in density-functional calculations is now standard practice in computational chemistry and materials science. In this talk, we review how the dispersion energy can be written as an asymptotic series expansion from perturbation theory, which can be added to the self-consistent energy. We then focus on the exchange-hole dipole moment (XDM) model, in which the dispersion coefficients are non-empirical and depend directly on the electron density and related properties. XDM offers simultaneous high accuracy for a diverse range of chemical systems, including binding energies of small molecular dimers, exfoliation energies of layered materials, and absolute and relative lattice energies of molecular crystals. Accurate and efficient computation of relative energies of molecular crystal polymorphs is of central importance for development of solid-state pharmaceuticals and is a requirement for first-principles crystal structure prediction (CSP). Several applications of XDM-corrected density-functionals for CSP are highlighted. Finally, we illustrate how candidate crystal structures from a CSP landscapes can be matched to experimental powder X-ray diffractograms, allowing identification of unknown polymorphs from solid-form screening studies.