

Department of Chemistry

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Location: Atrium AT101

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.

Biography:

Erin R. Johnson is originally from Ottawa, Canada and obtained her B.Sc. (Honours) at Carleton University. She completed her Ph.D. in chemistry at Queen's University in 2007, under the supervision of Prof. Axel Becke. She was then an NSERC post-doctoral fellow at Duke University in the group of Prof. Weitao Yang. Johnson is now a Professor at Dalhousie University, in Halifax, Canada, where she holds the Herzberg-Becke Chair in Theoretical Chemistry. She is also currently a Royal Society Wolfson Visiting Fellow at the University of Cambridge. Her research focuses on development and application of density-functional theory, with an emphasis on intermolecular interactions and molecular crystals. She has received numerous prestigious awards, including the



2021 Steacie Prize, the 2020 Rutherford Memorial Medal in Chemistry, a 2019 E.W.R. Steacie Memorial Fellowship, and the 2018 Dirac Medal.