

Midterm Seminar of Carl Frostenson

in [Fasrummet \(A820\)](#) between 13-14 on March 27th

Title

Range-Separated Hybrid vdW-DFs for Simple Structures and Complex System

Abstract

Are you curious about the latest advances in hybrid exchange-correlation functionals of the van der Waals density functional (vdW-DF) method here at Chalmers? This talk will delve into recent advancements and testing of analytical-hole range-separated hybrid (RSH) vdW-DFs, which utilize screening of the Fock-exchange component to provide improved characterizations of molecule, bulk, and surface systems.

I will focus on my work to test the progress of the vdW-DF description of metals, semiconductors, and oxide materials as well as show how it can be used towards present materials challenges by discussing my ongoing exploration of catalysis in a porous zeolite. For the former, I will discuss tests of a stress formulation for spin vdW-DF calculations. For the latter, a detailed account of the copper-oxide charge states is necessary, which motivates the use of the latest general-purpose RSH vdW-DF, termed vdW-DF2-ahbr.

Coffee and cake will served following the event