Introduction to Density Functional Theory Calculations and Applications in Catalysis

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Abstract

Electronic-structure methods are powerful tools for the prediction and rationalization of material properties. Given the good balance between accuracy and computational cost, Density functional theory (DFT) is among the most popular methods currently applied both in academia and industry.

In this seminar I will introduce the basics of DFT, starting from the Hohenberg-Kohn theorem, and I will show selected applications of this methodology to catalysis-related problems.