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Introduction to DFT and application to layered materials

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Density functional theory (DFT) is a successful theory to determine the electronic structure of atoms, molecules and solids. As a quantum chemical approach, its ultimate goal is the approximate solution of the Schrödinger equation. In the first part of the talk, I will provide a pedagogical overview of the main simplifications and fundamental theorems of this theory. Then, I will illustrate these concepts using the Quantum Espresso software package through its application to layered and 2D materials. In particular, we will focus on the gas sensing properties of WS2 in the presence of H2S, NH3, NO, CO and H2.

Time: 20 + discussion