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The quantum many-body problem and properties of materials: how to profit from machine learning?

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The understanding and prediction of properties of materials is a quantum many-body problem, and the observed phenomena often go well beyond the range that can be described with simple models. Recently, machine learning has emerged as a new tool that could potentially capture materials-specific or hidden universal features, and therefore help to analyse or design materials, and to improve theory.

The first part of this talk will introduce the domain of research and some typical questions, with special emphasis on spectroscopic properties. In a second part, we will concentrate on the design of density functionals to describe materials and give an example of our own research. Indeed, in the framework of Density Functional Theory (DFT), much effort is concentrated on finding the total ground state energy as a functional of the density, whereas other ground state expectation values are less studied. In this talk we will motivate the search for an expression for the one-body density matrix as a functional of the density. We will discuss strategies to develop approximations, and the multiple role that machine learning can play in this context [1,2].

[1] A. Aouina, M. Gatti, and L. Reining, Faraday Discussions 2020, 224, 27
[2] J. Wetherell, A. Costamagna„ M. Gatti, and L. Reining, Faraday Discussions 2020, 224, 265

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