**DFT and machine learning for quantum materials**

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**Abstract:** In recent years, density functional theory (DFT) and machine learning (ML) have transformed many scientific fields, including materials science and physics. DFT is a powerful tool for studying quantum materials because it can directly calculate their properties without relying on experimental parameters. However, DFT involves costly calculations, often requiring the use of supercomputers. Therefore, it is not ideal for screening methods or for handling complex and large systems. Nevertheless, ML offers a new approach to studying quantum materials with high accuracy while being much faster than DFT. In this talk, first, we will briefly introduce the DFT and our study project on this, as such thermoelectricity, Raman, optic [1,2,3], and second, we will introduce a new ML architecture featuring universal embedding, the so-called GNNOpt [4], which can predict the optical properties of materials from crystal structures only. The model performs a highly precise optical prediction at the DFT level, making it suitable for various applications, from solar cells to quantum materials.

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