Application of optimisation methods in computational materials science

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Abstract: Optimization techniques are at the heart of computational schemes used to model materials and their physical properties. In this talk, I will present three basic applications of optimization methods in the fields of materials science and physics. The first and second applications, are interconnected and deal with topology optimisation of molecular or solid structures and the calculations of their electronic properties through quantum mechanics. These calculations require the application of optimisation methods such as the Broyden-Fletcher-Goldfarb-Shanno algorithm and the resolution of the self-consistent-field problem. Showcase examples such as the study of defects in semiconductor materials [1, 2], the calculation of magnetic properties of 2D materials [3] and the study of cathode materials for Na batteries [4] will be briefly presented. The third application deals with the development of machine learning interatomic potentials based on the Gaussian process regression. This scheme allows one to accurately map a complex and high-dimensional potential energy surface of a given material and consequently enables the possibility of modelling large systems with thousands of atoms at a negligible computational cost [5].

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