Material-design using ab-initio theory

tutorial

August 21, 2019 | 4:00 pm
Lecture Hall MPI | B.1.11

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Abstract

The development of density-functional theory in the 1960s and the dissemination of computers led to a revolution in materials science. A third kind of physics, computational physics, emerged to complement its theoretical and experimental sisters. By solving complex theoretical models in a computer we had access to quantitative results for specific systems. These numerical experiments could explain experiments or be used to predict new materials and their properties.

Nowadays, with the availability of ever faster supercomputers and novel computer methodologies, we are living what I would call the second computer revolution in materials science. High throughput techniques, together with ever faster supercomputers, allow for the automatic screening of thousands or even millions of hypothetical materials to find solutions to present technological challenges. Moreover, machine learning methods are used to accelerate materials discovery by replacing density-functional theory by extremely efficient statistical models.

Speaker

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