Response properties of inorganic materials from high-throughput density-functional perturbation theory and machine-learning

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The progress in first-principles codes and supercomputing capabilities have given birth to the so-called high-throughput (HT) ab initio approach, thus allowing for the identification of many new compounds for a variety of applications. A number of databases have thus become available online, providing access to properties of materials, mainly ground-state though. Indeed, for more complex properties (e.g., linear responses), the HT approach is still problematic because of the required CPU time. To overcome this limitation, machine learning approaches have recently attracted much attention.
In this talk, I will review recent progress in materials informatics focusing on the response properties of inorganic materials which play of key role in various physical phenomena such as linear and non-linear optics, thermal conductivity, superconductivity, or ferroelectricity. I will first present our HT calculations of the response properties based on density functional perturbation theory. I will briefly introduce the OPTIMADE API that was developed for searching the leading materials databases using the same queries. Finally, I will review the MODNet framework for predicting materials properties and which is particularly well suited for limited datasets through the selection of physically meaningful