Automated in silico design of materials for energy and plasma applications

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Abstract: Materials and their properties play a vital role in most applications we use on a daily basis. During the past few decades, computational materials science has started evolving more and more into a predictive tool instead of simply offering theoretical insight into the physical processes of materials of interest. In combination with increasingly available tools for automating the required calculations, this has led to the concept of in silico materials design, where large numbers of compounds are investigated using computer simulations in order to gauge their potential for a specific application. Among the most successful theoretical frameworks for computational materials science is density functional theory, which can determine the electronic structure of many compounds with ever increasing accuracy using a reasonable amount of computational resources. However, the connection between the electronic structure of a material and the property of interest for a specific application is rarely trivial. The main goal of my work is to provide or improve this connection, by analyzing existing metrics for flaws or anomalies, and developing new descriptors of material properties as well as the tools for calculating them using automated workflows. These methods are then applied to a set of topics including solar cells, Li-ion batteries and ion-induced secondary electron emission.