Inverse Materials Design for Tungsten Alloys

It is about 25 years since density-functional theory has become applicable with sufficient accuracy to real materials. This quarter of a century of expertise has enabled the DFT community to gain a good insight in the strength and weaknesses of DFT predictions. The community is now clearly evolving from explanatory to predictive studies, with "computational materials design" as the often-promised ultimate goal.

In this contribution, we will discuss how to quantify the expected accuracy of DFT-predictions. Only when knowing the "error bar" on DFT predictions, computational materials design efforts make sense [1].

Not all materials design problems are equally suited for a computational (DFT) approach. We will spend some thoughts on the question "to which kind of design questions DFT can make useful contributions?". We will identify some of these questions in the context of materials development for nuclear fusion applications (post-ITER), and we will report on a case study in which a computational strategy is used to narrow the search space for candidate materials (i.c. tungsten alloys) for the first wall of fusion reactors.

[1] K. Lejaeghere et al., "Error estimates for solid-state density-functional theory predictions: an overview by means of the ground-state elemental crystals", http://arxiv.org/abs/1204.2733v3, to appear soon in Critical Reviews in Solid State and Materials Sciences.