An extended Pareto approach to computational materials design: tungsten alloys for nuclear fusion reactors

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Resume : Because of competing design criteria, it is often hard to decide on one particular material as the best solution for a given need. A multidimensional optimization strategy can already narrow down the initial large set of candidates to a much smaller number of promising materials, the Pareto-optimal set. Quite often, however, this set contains more materials than can be afforded for further systematic examination. An ordering within this set, highlighting the most promising candidates, would be very useful to expedite the design process. Conventional Pareto approaches cannot offer such a ranking. We present an algorithm to do exactly this [1]. This procedure is applied to a set of binary and ternary tungsten alloys to look for a candidate first-wall material for nuclear fusion purposes [1, 2]. Because of the harsh operating conditions inside (future) fusion reactors, materials selection is a critical aspect there. Tungsten is a promising first-wall material, but several issues, such as room-temperature brittleness, are still to be resolved. Alloying tungsten with other elements is one possible way of overcoming these problems. By combining a computational screening study (at the DFT-PBE level) with our extended Pareto analysis, a select number of alloys is presented as most promising candidates for further experimental investigation. [1] K. Lejaeghere et al., Phys. Rev. Lett. 111, 075501 (2013). [2] K. Lejaeghere et al., Phys. Rev. B (2014), accepted.