

Picking a Rolex out of a box of Swatches: high-throughput calculations with Pymatgen

Vincenzo Fiorentini

University of Cagliari and CNR-IOM

The design of new materials has traditionally been an artisan endeavor where painstaking attention to detail is key (akin, one would like to imagine, to producing a high-end watch as opposed to a mass-produced trivial one). Recently, it has become possible, and useful, to orient the search for such focused work using search and interrogation of large databases of (mostly generic) materials properties, possibly automated and machine-learning-driven. I will discuss a few applications originating from one of the environments currently in vogue for this kind of work, the PyMatGen tool for searching and extending the Materials Project database.

Vincenzo Fiorentini is associate professor at Cagliari University, Italy. He works in the general area of theoretical (mostly ab initio) solid-state and materials physics.