High-throughput studies in computational solid-state physics: a review

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While high-throughput studies are a relatively recent development in the context of materials science as a whole, they are also mature enough that a set of defining traits can be identified. This contribution aims to provide an overview of the field including its history, features, main achievements and most important open challenges.

The starting point is a review of the earliest attempts at high-throughput studies of solid-state systems, but more importantly of their notable predecessors in theoretical chemistry. This is followed by an analysis of the factors that made the current wave of high-throughput research possible.

On this background, the talk then presents a sketch of the main ingredients that define high-throughput studies in our field today. Special emphasis is put on the largest international projects that have emerged as a natural consequence of those general ideas. A small survey of studies showcasing the implementation and consequences of this approach are discussed in some detail.

The last part of the talks deals with the main barriers to further development of high-throughput studies, from both a scientific and a technical perspective, and with the sometimes tense relationship with conventional attitudes in material science.