Accelerating materials’ discovery with evolutionary algorithms in chemistry

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Abstract

This talk provides an overview of the computational tools that we recently developed in our group to help and support our experimental partners in the discovery of porous materials and polymers for energy generation. Specifically, I will address the biggest obstacles encountered in the experimental design of new materials and how computational chemistry can be applied to accelerate this process. Furthermore, I will introduce the concept of evolutionary algorithms and how these approaches can be used in material science to efficiently probe a huge chemical space and suggest sensible candidates for the direct experimental synthesis. Evolutionary algorithms are inspired by Darwin's theory of evolution and pit candidate materials against each other as with the "survival of the fittest" in nature. Each generation of candidates is tested with simple calculations that predict their properties as a measure of their fitness. The fittest candidates are most likely to survive to the next generation, but also random mutations of their features will occur and pairs of candidates will parent new offspring with mixtures of their features - just as occurs in nature. Finally, I will present our latest results showing the wider applicability of the method to new chemical systems and prove how computational modelling can be responsible for the discovery of new materials with useful applications, rather than simply rationalizing results from synthetic teams.