Billions and Billions of Molecules

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Many of the challenges of the twenty-first century are related to molecular processes such as the generation and storage of clean energy, water purification and desalination. These transformations require a next generation of more efficient, chemically stable, and non-toxic materials. Chemical space, the space of all possible synthesizable molecules, is practically infinite and promises to have relevant candidate functional molecules to address these challenges. One of the main goals of my research group is to develop understanding and tools for the exploration chemical space in order to accelerate the discovery of organic materials. Our design cycle is sped up by the constant interaction of theoreticians and experimentalists, the use of high-throughput computational techniques, machine learning, and the development of specialized big data tools. We have had recent successes in theoretically predicting and experimentally confirming in record times top performers in the areas of organic electronics, organic flow batteries and organic light-emitting diodes. In this talk, I will discuss what I consider are the key factors related with a successful high-performance screening approach as illustrated by these three different applications. I will end by discussing the future prospects and challenges associated with developing appropriate metrics for the cartography of chemical space.