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Construction of a Ready-to-Use Database to Enable Accurate High-Throughput Screenings of Covalent Organic Frameworks

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Covalent organic frameworks (COFs) [1] are a new class of crystalline nanoporous materials. They consist only of light atoms and are held together by strong covalent bonds, which result in an exceptionally high mechanical, thermal, and chemical stability. This makes that these COFs are particularly interesting for industrial applications such as carbon capture [2]. According to the concept of reticular chemistry, COFs can be decomposed into building blocks, in the same manner as metal-organic frameworks [3]. Recombining these building blocks in alternative patterns allows for the construction of new, hypothetical COF materials (see Figure). This approach results in an almost unlimited number of structures that can possibly be synthesized, which makes that an experimental screening to characterize this class of materials is beyond our reach. In the past decades, computational techniques have evolved to the point where efficient high-throughput screenings become feasible, bypassing the need to experimentally synthesize these materials. Besides the faster identification of promising candidates for industrial applications, this approach can also reveal the performance limits of COFs and establish interesting property-property relations [4].

In this work, we have constructed a ready-to-use database of both experimentally observed and hypothetical COFs, taking into account the large variety of possible structures, together with a QuickFF force field [5] for each material. To generate the geometrical structures, a top-down approach is followed [4]. Starting from a topology in the RCSR database [6], appropriate building blocks are placed on its vertices to form periodic structures. As each structure in the database is provided in an energy minimum, the materials in this database can immediately be adopted in molecular simulations with the given force field, allowing for the possibility to perform high-throughput screenings of COFs in a computationally feasible way.

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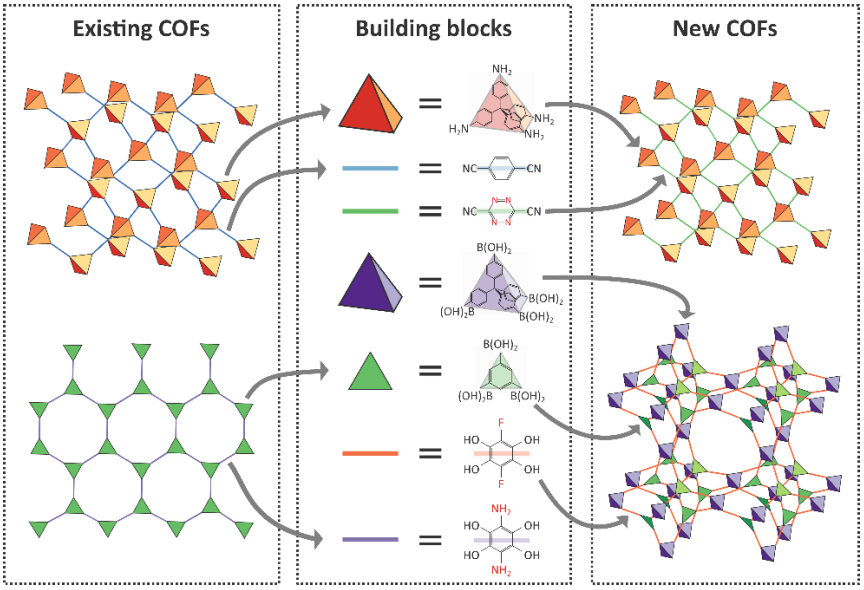

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