Automated MOF discovery platform for clean energy applications

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Metal/covalent-organic frameworks (MOFs) are crystalline, nanoporous materials composed of (in)organic nodes connected by organic linkers. Because of their highly tunable structure, high porosity, and large internal surface area, MOFs are of great interest for various applications such as catalysis, gas separation, and gas storage. The multitude of nodes, linkers, and functional groups can be combined to form a vast array of plausible MOF structures. The chemical space of all possible MOFs is far too large to thoroughly sample using brute force; therefore, we must turn to automated search methods to identify promising candidates tailored for a specific application. We designed a hybrid variational autoencoder (VAE) for the automated design of novel MOFs and trained it with known MOF structures. MOF structures are automatically decomposed into their building block sequence (linker+node+topology), and a graphic-based junction-tree pre-VAE is used to learn and predict new linkers and nodes while a sequence-based VAE is used to learn and predict new building block sequences with the optimization guided by the calculated properties of previously generated MOFs. We utilize the hybrid VAE and for different applications, train the hybrid VAE with corresponding properties and predict MOFs with improved performance.