Computational screening of metal-organic frameworks for adsorption heat pumps

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Adsorption heat pumps(AHPs) driven by low-grade heat sources including waste heat and solar energy is promising for heating and cooling. However, the coefficient of performance (COP) of AHP is unsatisfactory due to the low uptake and high regeneration cost of conventional adsorbents. Metal-organic frameworks (MOFs) were recognized as potential adsorbents due to their outstanding properties. However,it is a challenging task to quickly find out the potential candidates from a huge number of MOFs. In this work, high-throughput computational screening[1,2] was employed for evaluating the heating/cooling efficiency of a large number of MOFs [3]. Structure-property relationship highlighted the importance of pore size, shape of adsorption isotherms and Henry's constant towards working fluids in determining COP. Machine learning algorithm was successfully carried out to predict the COP of MOFs. This work provided useful insights into the exploration of high efficient AHPs based on MOFs.