Inverse Design of Metal-Organic Frameworks with User-desired Xe/Kr Selectivity and Xenon Henry coefficient

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Inverse design of materials is defined as the workflow to create materials that cater towards the user-desired input. So, the workflow can guarantee a significant level of efficiency to design specific materials. Its high efficiency in materials design field is especially helpful to design metal-organic frameworks (MOFs) because countless MOFs can be synthesized with various different combinations of tunable building blocks. In this work, we designed user-desired MOFs by using a validated platform that integrate genetic algorithm with machine learning. We presented xenon related adsorption properties such as xenon/krypton selectivity and xenon henry coefficient as inputs. First, we obtained two candidates with record-breaking xenon/krypton selectivity that show significant improvement over the current record through our platform. Furthermore, we prove that our platform can be extended to design MOFs which satisfy the specific desires of the users across multiple properties and range of property values with the simple modification in the cost function of genetic algorithm.