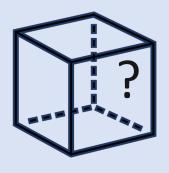# I. Rapid screening pipeline to find highly selective materials

Unknown 3D MOF
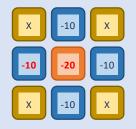
?

Preliminary geometrical evaluation
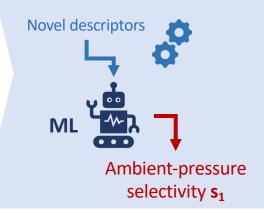
LCD

Zeo++

Pre-evaluation infinite dilution selectivity

X	-10	X
-10	-20	-10
X	-10	X

C++

Final ML evaluation

Novel descriptors

ML

Ambient-pressure selectivity s_1

II. Higher level evaluations on the promising materials

Adsorption properties   **GCMC calculations**   **Data analysis**   **MOF synthesis**   **Experimental properties**