Overview of PrISMa Submission

Submission

Key	Value
Name	Joren Van Herck
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Position	PostDoc
Submission time	2023-08-10 09:37
Structure Name	TEST
Submitted cif	HKUST1_exp.cif

Model Predictions

The structure is extracted from the CIF file and cleaned with c2x. This extra step was needed to create a Persistence Homology Images (PHImages), a descriptor related to the pore geometry. The PH image was used to predict (i) the Net Carbon Avoidance Cost relative to the MEA-based benchmark and (ii) the water resistance. Both models where trained for the cement case in the UK with TSA process.

Model Name	Input Type	Prediction	Explanation
nCAC	PHImage	0	whether a material has a lower nCAC than the MEA-based benchmark
WaterResistance	PHImage	1	whether a material can maintain its CO_2 adsorption capacity in wet flue gasses