

【CL2-1】

Investigating porous material with persistent homologySenja Barthel¹, Paweł Dłotko², Kathryn Hess³, Yongjin Lee¹, S Mohamad Moosavi¹, Berend Smit^{1,5}

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Material science is a field with many potential applications of persistent homology. Many properties of materials are related to shapes, for example the arrangement of atoms or that of potentials or densities. The talk will show the construction of a persistent homological descriptor for pore shapes of nano-porous materials to examine geometric similarities of these materials. This allows drawing conclusions on the material's gas adsorption and separation behaviour, in particular carbon capture and methane storage.

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