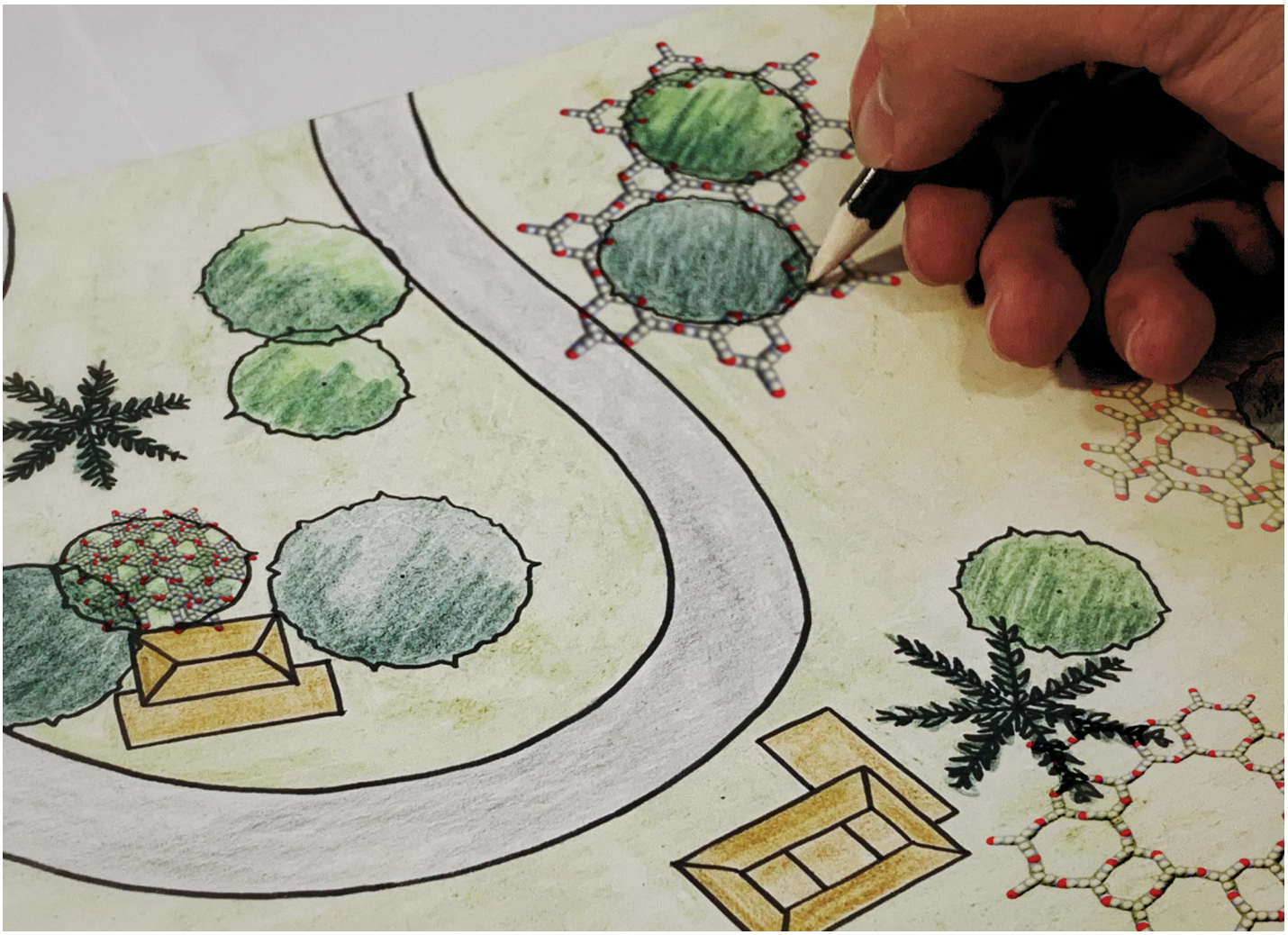

Showcasing research from Professor Smit's laboratory, Institute of chemical sciences and engineering (ISIC), École Polytechnique Fédérale de Lausanne (EPFL), Valais, Switzerland.

Geometric landscapes for material discovery within energy–structure–function maps

Geometric landscapes are introduced to represent the complex energy-structure-function maps of porous molecular crystals. This representation is based on the similarity of the pore geometry of the materials quantified using persistent homology, a mathematical tool from topological data analysis. We used geometric landscapes and machine learning to explore datasets of porous molecular crystals and successfully identified the energetically favourable and functionally interesting polymorphs among the 1000s to 10,000s of structures in each dataset. This novel representation aids in screening and exploring for high performing porous materials.

As featured in:

See Berend Smit *et al.*, *Chem. Sci.*, 2020, **11**, 5423.

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