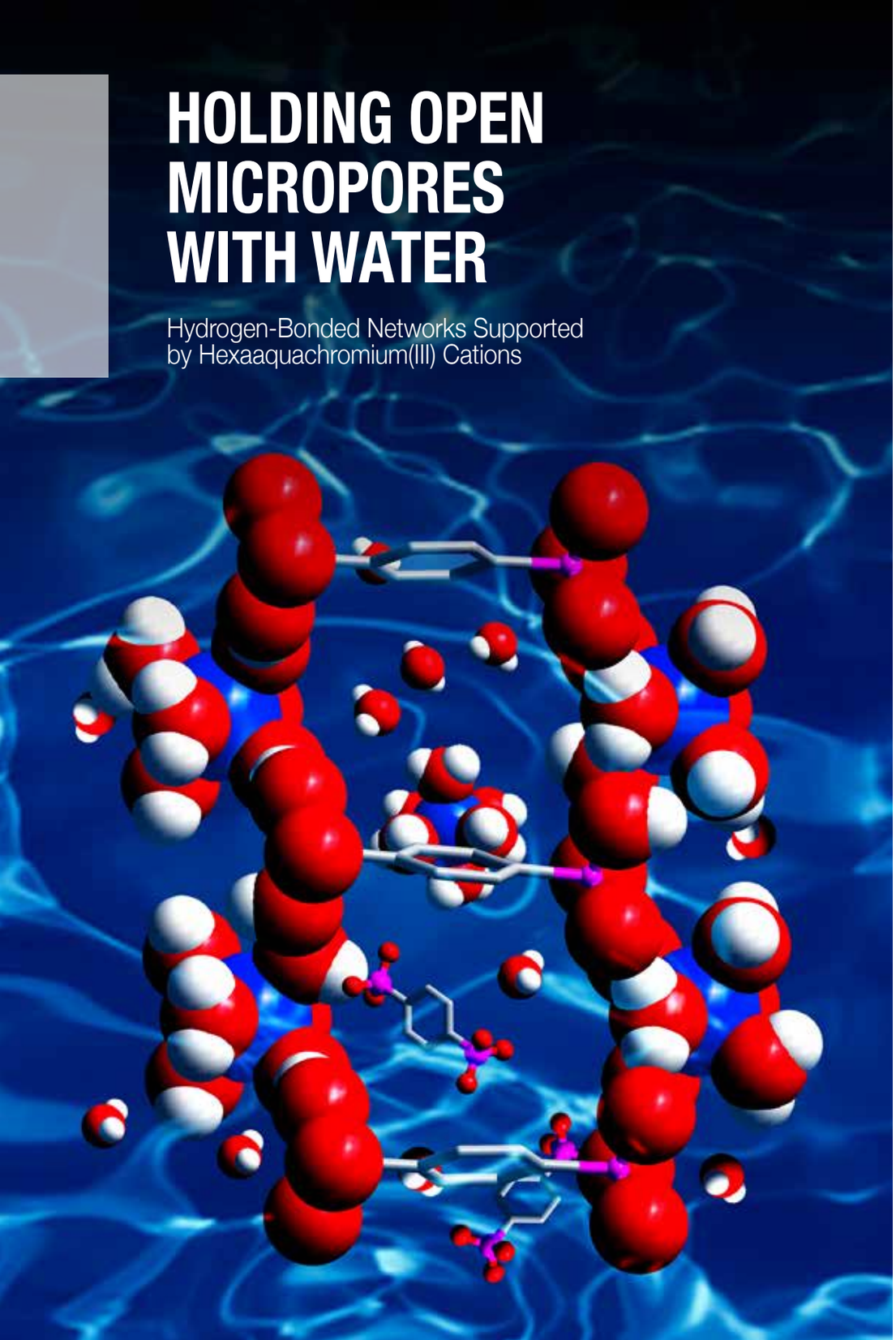
HOLDING OPEN MICROPORES WITH WATER

Hydrogen-Bonded Networks Supported by Hexaaquachromium(III) Cations



Jared Taylor & George Shimizu use X-ray Diffraction to characterize the behaviour of porous solids.

Porous solids are materials that contain cavities, channels, or interstices. Depending on the size and shape of the pores and the chemical surfaces lining them, they can be used for applications ranging from separations and catalysis to sensing and delivery vessels.

Many of the newer classes of porous solids such as metal-organic frameworks (MOFs), covalent organic frameworks (COFs), polymers of intrinsic microporosity (PIMs), porous aromatic frameworks (PAFs), and porous molecular cages can be modified so as to tune the chemistry and engineering behavior of these materials.

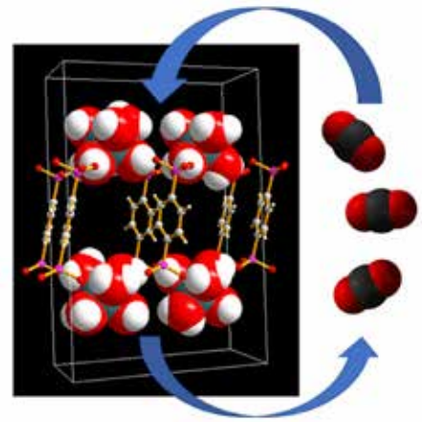
At the University of Calgary, George Shimizu's group makes new nanoporous solids, primarily metal-organic frameworks (MOFs), directed by applications in gas separations and ion conduction.

There are challenges to engineering these porous materials. "From surface enthalpic considerations, a void in a solid is always unfavorable," says Shimizu. There is an energetic penalty in forming a void and thus strong bonding and interactions play an important role in enabling pores to exist in these materials.

A second feature for modifying the performance of porous materials is order. Regular pore sizes and geometry give more predict able performance for adsorption and helps develop structure-property relationships. Weaker bonds such as hydrogen-bonds can form porous solids, provided sufficient complementarity and cooperativity exist between assembling partners.

A new family of hydrogen-bonded porous solids was discovered and developed by the Shimizu group (CHEM, 2018, 4, 868-878)". These solids demonstrate reversible gas uptake in their pores and, owing to the hydrogen-bonded structure, can also show dynamic structures where pores open and close, like a gate, in response to the concentration/pressure of what is being adsorbed.

Along with the team at PROTO, research associate Dr. Jared Taylor, demonstrated this unusual feature occurred in a hexaaquachromium phosphonate structure where pore "gating" was observed at elevated pressures of CO_2. In-situ



monitoring of the unit cell expansion at elevated CO_2 pressure was done using a PROTO AXRD Benchtop diffractometer outfitted with a pressure cell. This type of behaviour is unique to more weakly bonded solids and offers new avenues for smart sorbents and sensors.