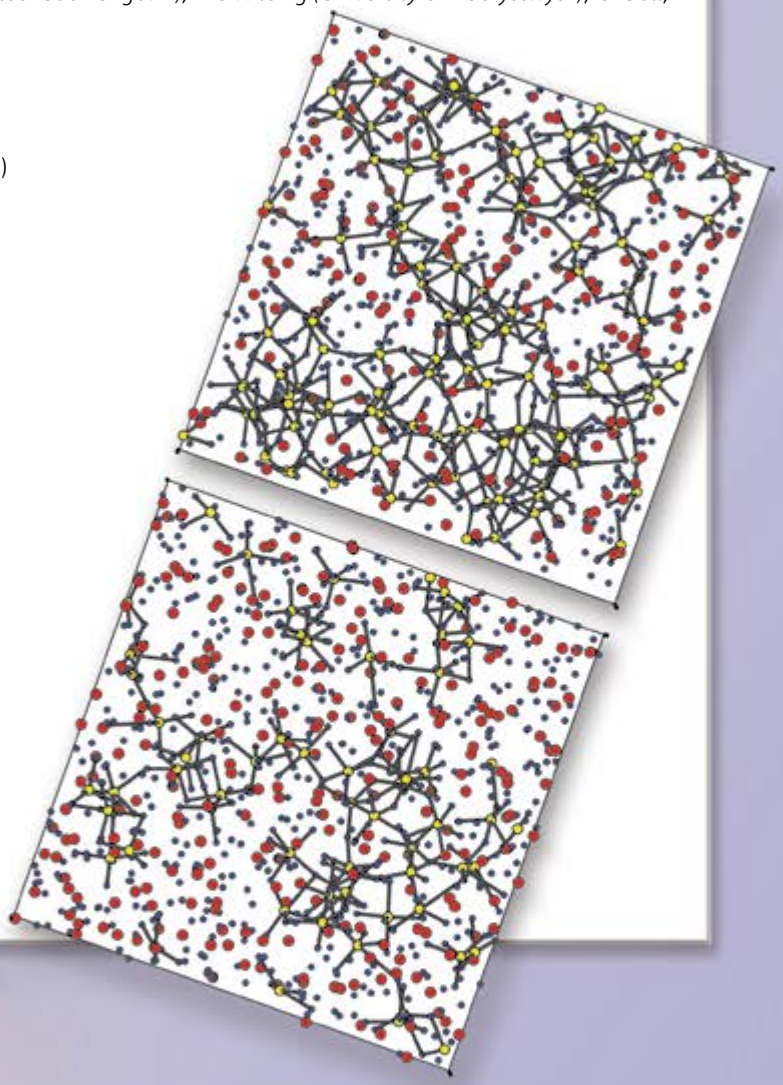
Rock *and ice*

Networks under pressure

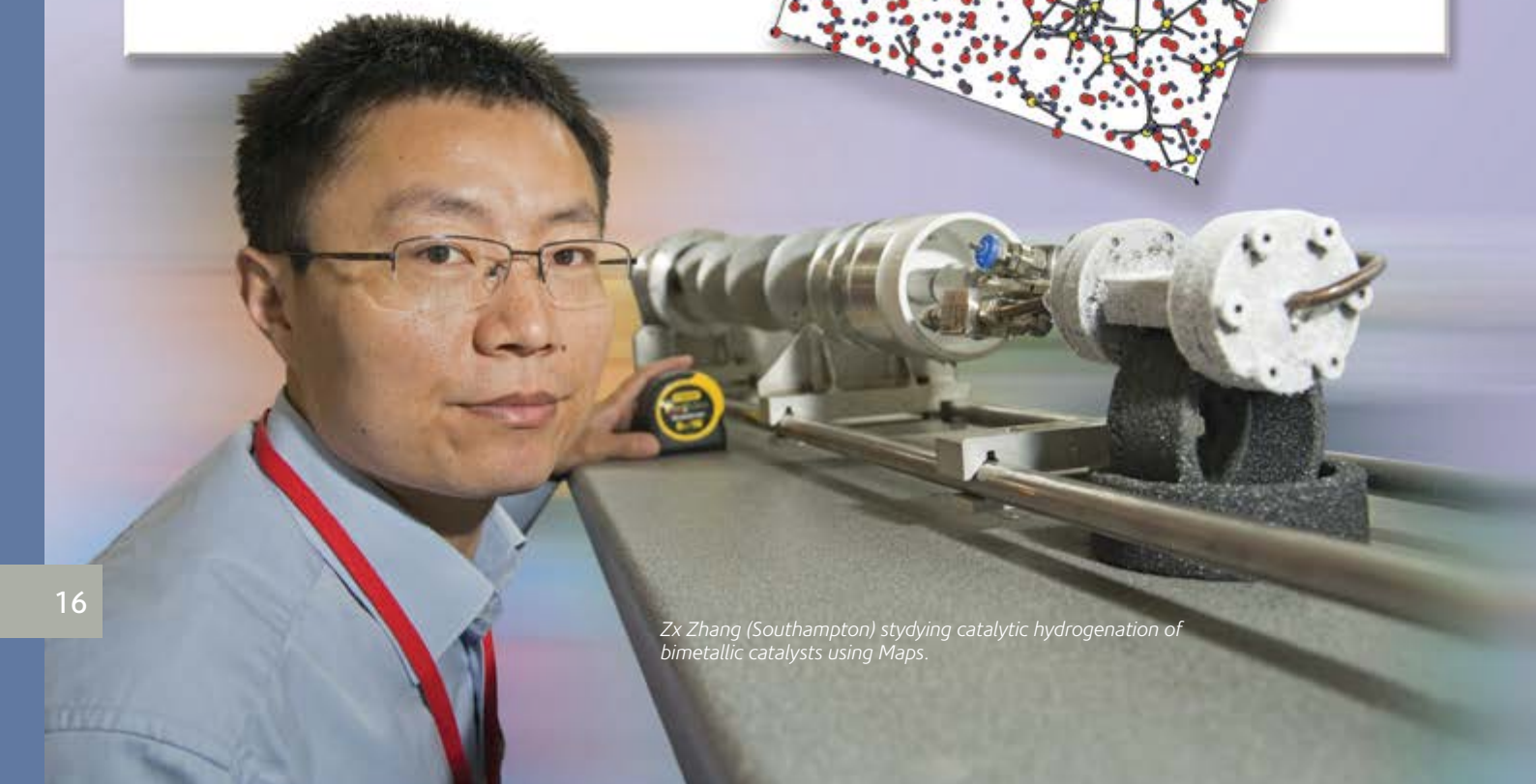
A Zeidler, K Wezka, RF Rowlands, DAJ Whittaker, PS Salmon, A Polidori (University of Bath), JWE Drewitt (University of Edinburgh), S Klotz (Université Pierre et Marie Curie, France), HE Fischer (Insitut Laue-Langevin), MC Wilding (University of Aberystwyth), CL Bull, MG Tucker (ISIS), M Wilson (University of Oxford)

Instruments: Pearl, D4c (ILL).
Research support: EPSRC, University of Bath, ILL.
Contact: Philip Salmon, P.S.Salmon@bath.ac.uk
Further information: A Zeidler et al., Phys. Rev. Lett. 113 (2014) 135501.

Silica is a major component in the sand on a beach and in the rocks below our feet, pointing to its widespread abundance on Earth. As a glass, the material is exploited to make the fibres used for optical telecommunication systems, and its behaviour under pressure serves as a reference for geophysically relevant silicates. At ambient conditions, the atomic-scale structure is built from a network of corner-sharing SiO_4 tetrahedral motifs that link to form open ring-like arrangements. But how does this network respond when high pressures are applied? We investigated this issue by combining neutron and X-ray diffraction experiments with molecular dynamics computer simulations. The results show that the network collapses via a process in which rings are 'zipped' by a pairing of higher-coordinated Si atoms, namely those at the centres of the SiO_5 and SiO_6 motifs that are coaxed into existence. The work provides a starting point for predicting how such changes to a network's connectivity govern its physical properties.



Right: As the pressure on SiO_2 glass is increased (bottom to top), 4-fold coordinated Si atoms (red) convert to 5-fold coordinated Si atoms (yellow) that cluster together.



Zx Zhang (Southampton) stydying catalytic hydrogenation of bimetallic catalysts using Maps.