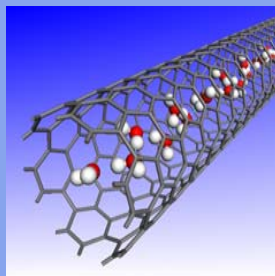
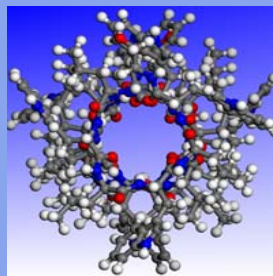
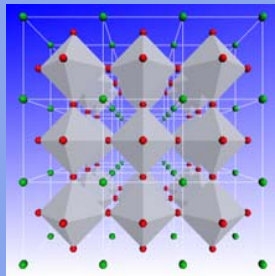
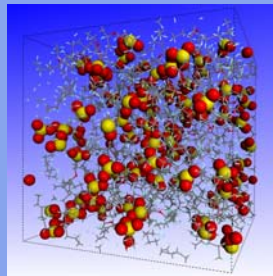


Overview and scope of meeting

11/4/2005

“Proton conduction in diverse media”

Fitzwilliam College, 11-12th April 2005



James Elliott

Materials Modelling Group

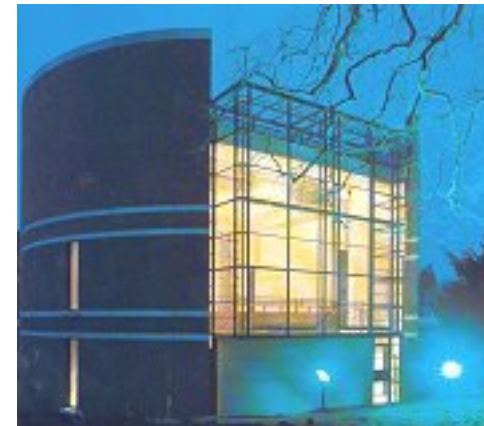
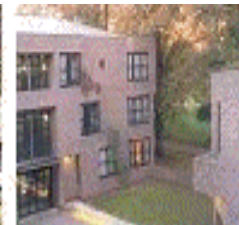
Department of Materials Science & Metallurgy

Stephen Paddison

University of Alabama in Huntsville



Fitzwilliam College, Cambridge



Acknowledgements for funding support

- The meeting supported by following bodies:
- UK Engineering and Physical Sciences Research Council (EPSRC) under GR/S80455/01

<http://www.epsrc.ac.uk>

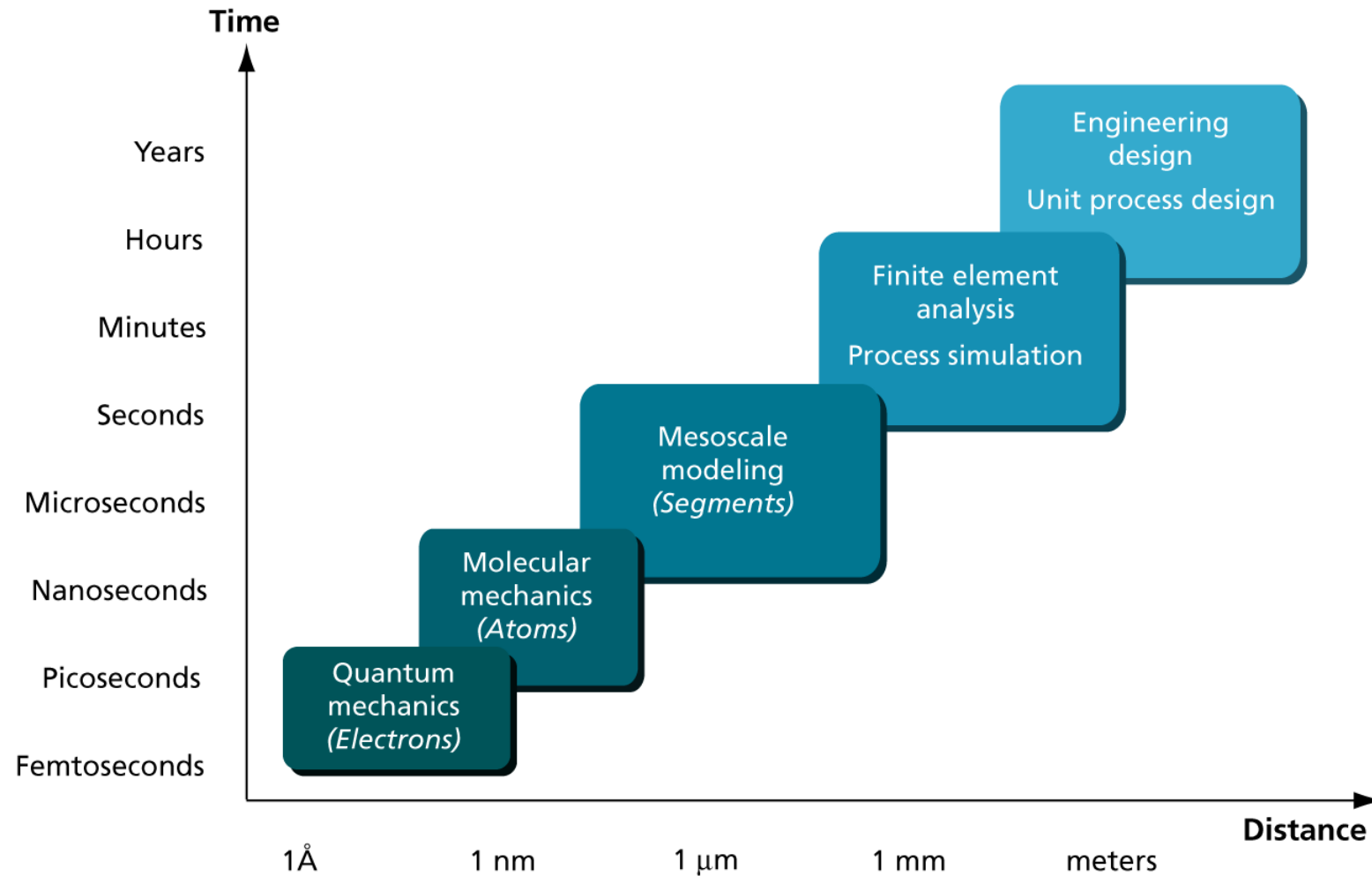


- UK Collaborative Computing Project number 5 (CCP5)
“... for computer simulation of condensed phases”

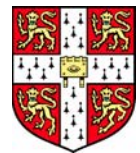
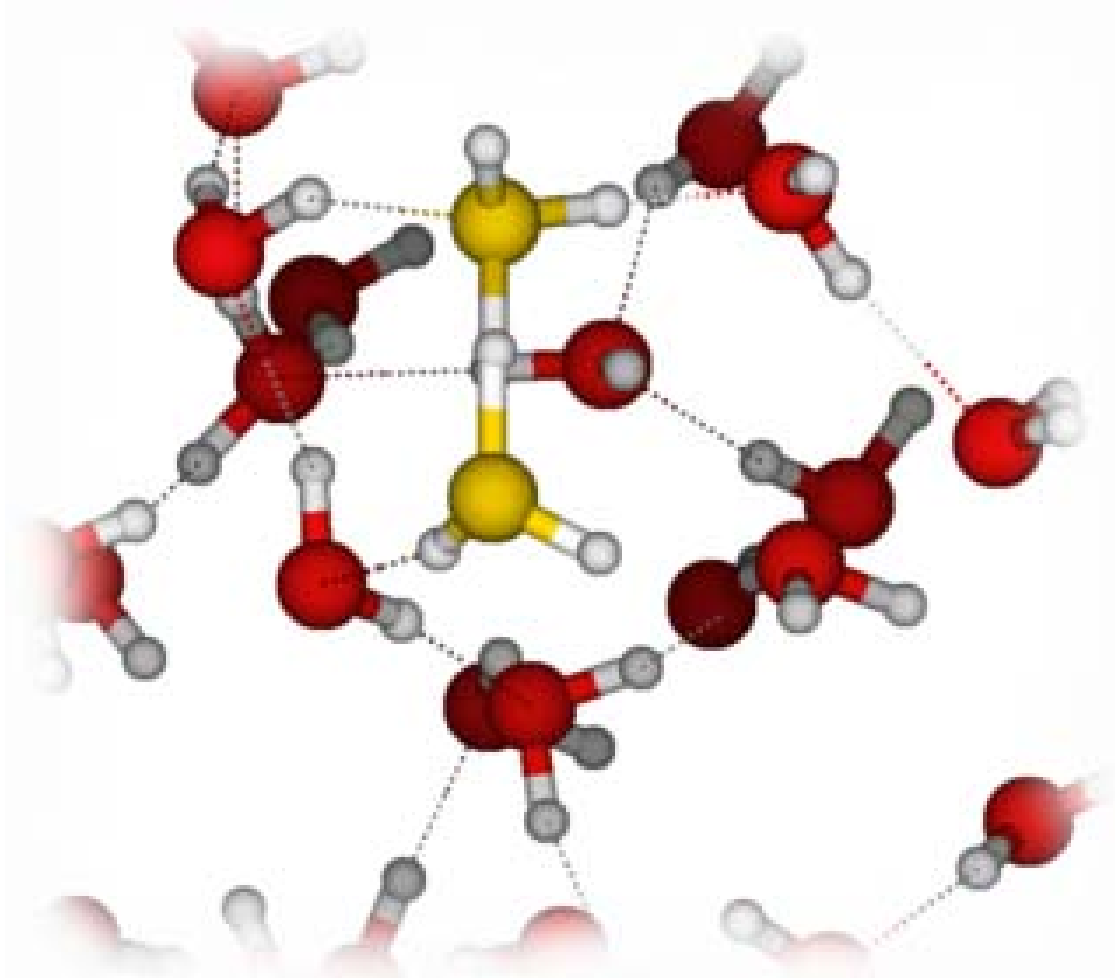
<http://www.ccp5.ac.uk>



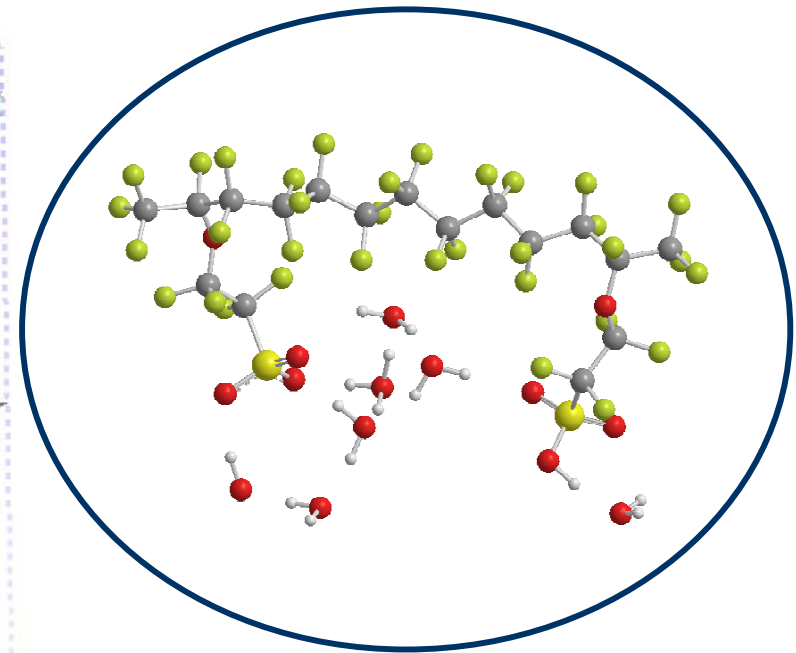
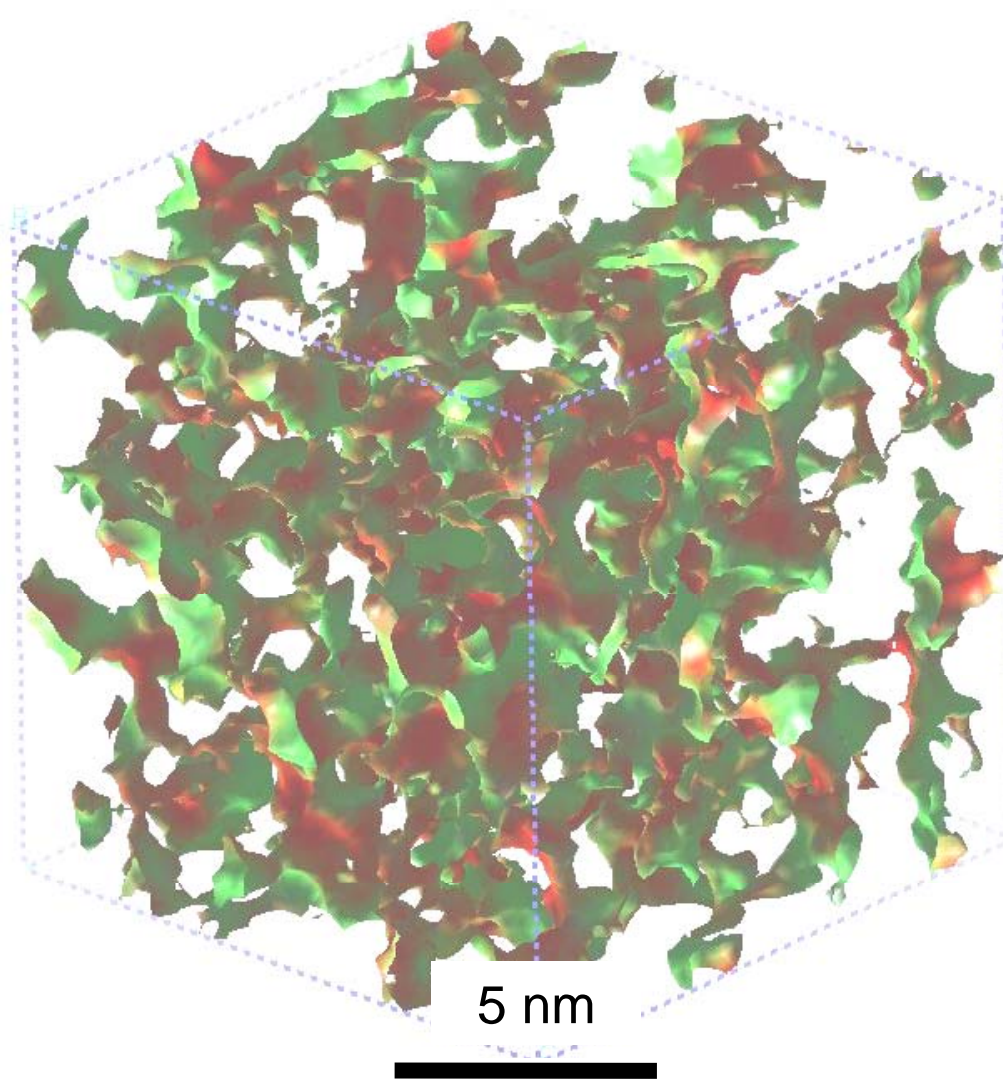
Multi-scale approach



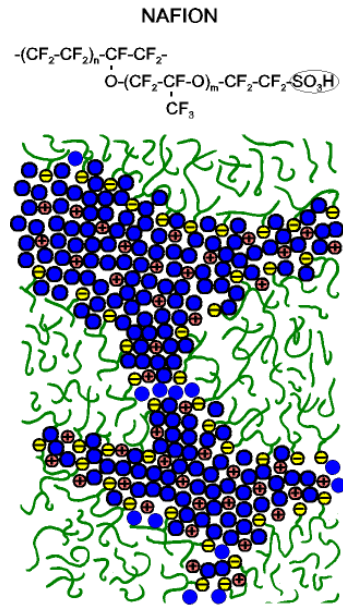
Proton transport in bulk water



Polymer electrolyte membranes for fuel cells



New membrane materials and composites

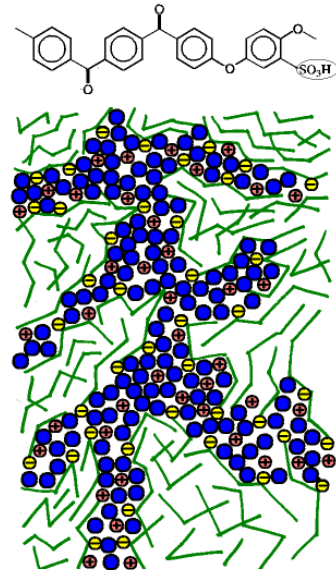


- wide channels
- more separated
- less branched
- good connectivity
- small $-SO_3^- / -SO_3^-$ separation
- $pK_a \sim -6$

relevant scales and interactions

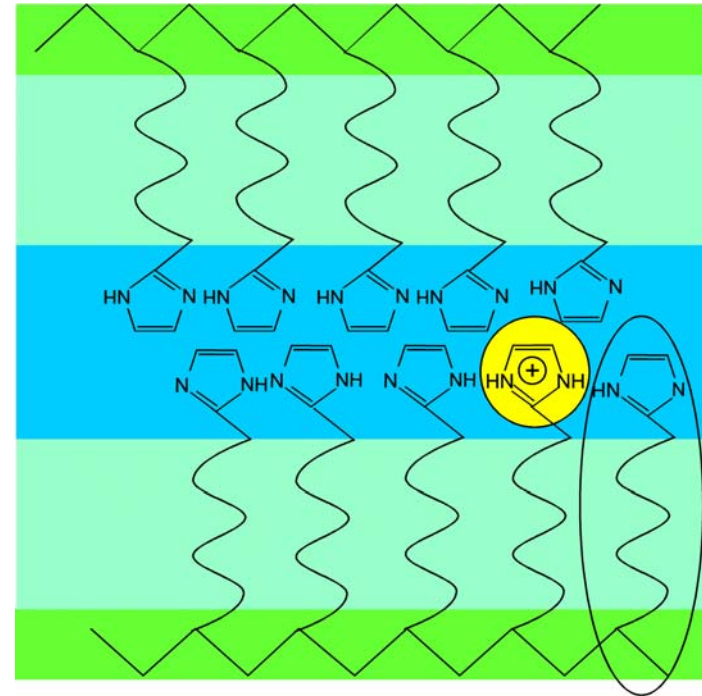
- 0,1 nm
- 1 nm
- 10 nm

sulfonated polyetherketone (PEEK)



- narrow channels
- less separated
- highly branched
- dead-end channels
- large $-SO_3^- / -SO_3^-$ separation
- $pK_a \sim -1$

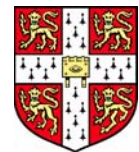
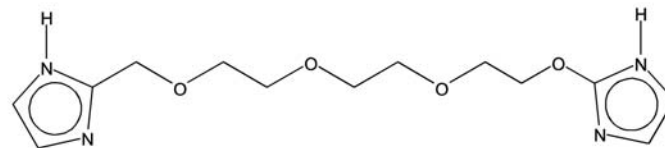
reactions on molecular scale
space charge effects (electrostatics)
percolation



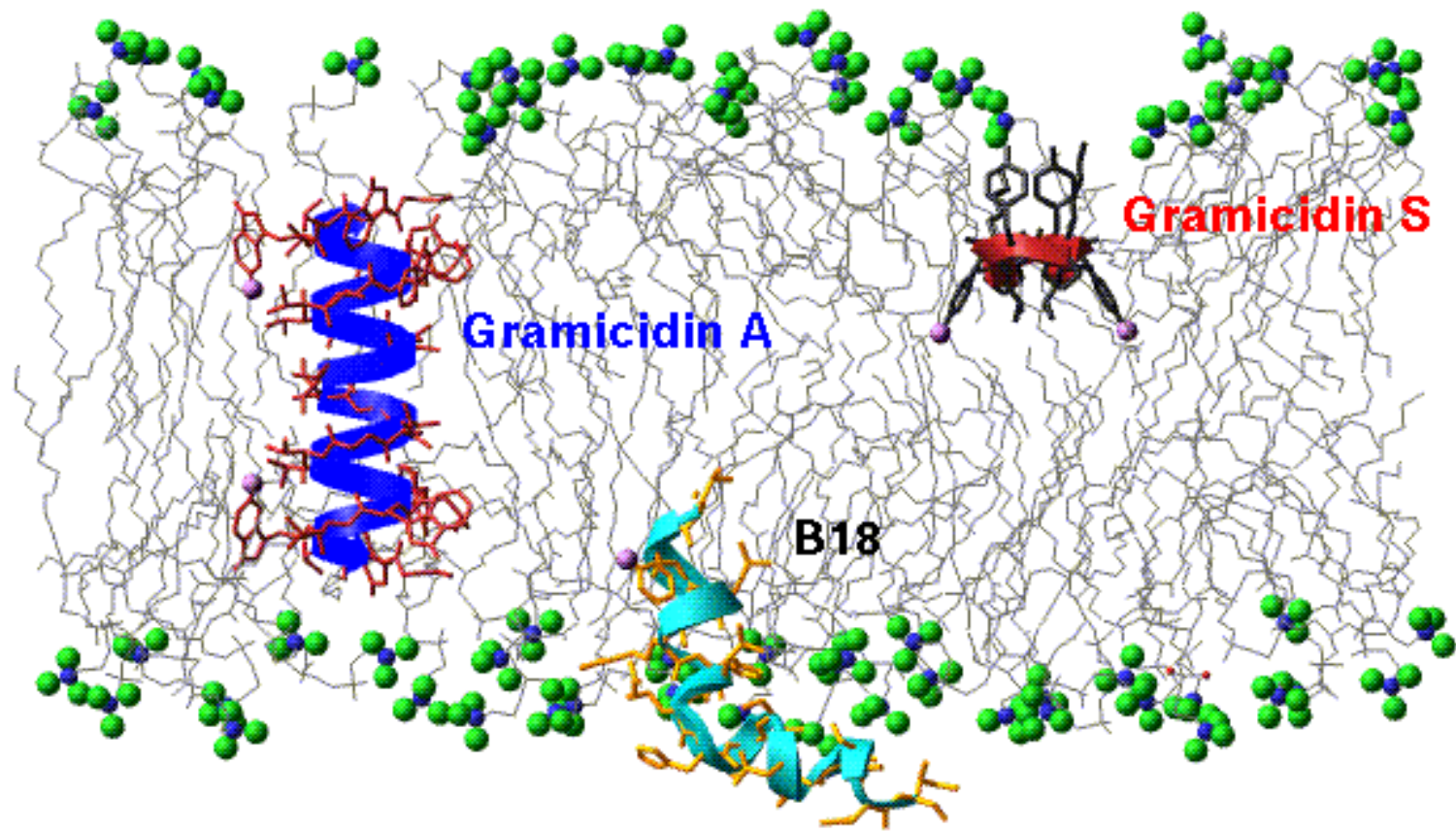
rigid polymer backbone

soft spacer

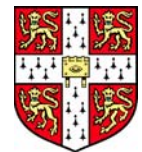
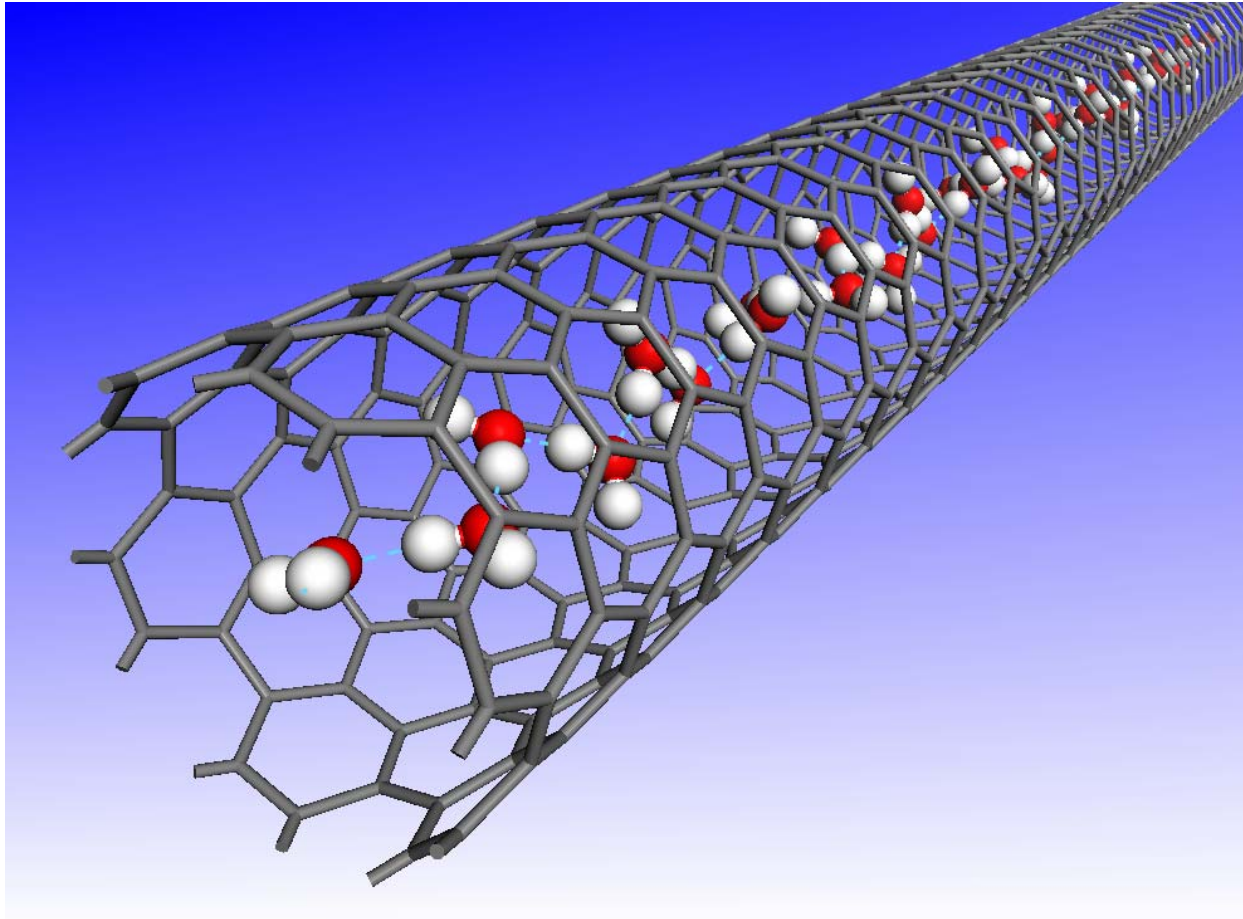
liquid - like proton solvent



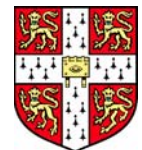
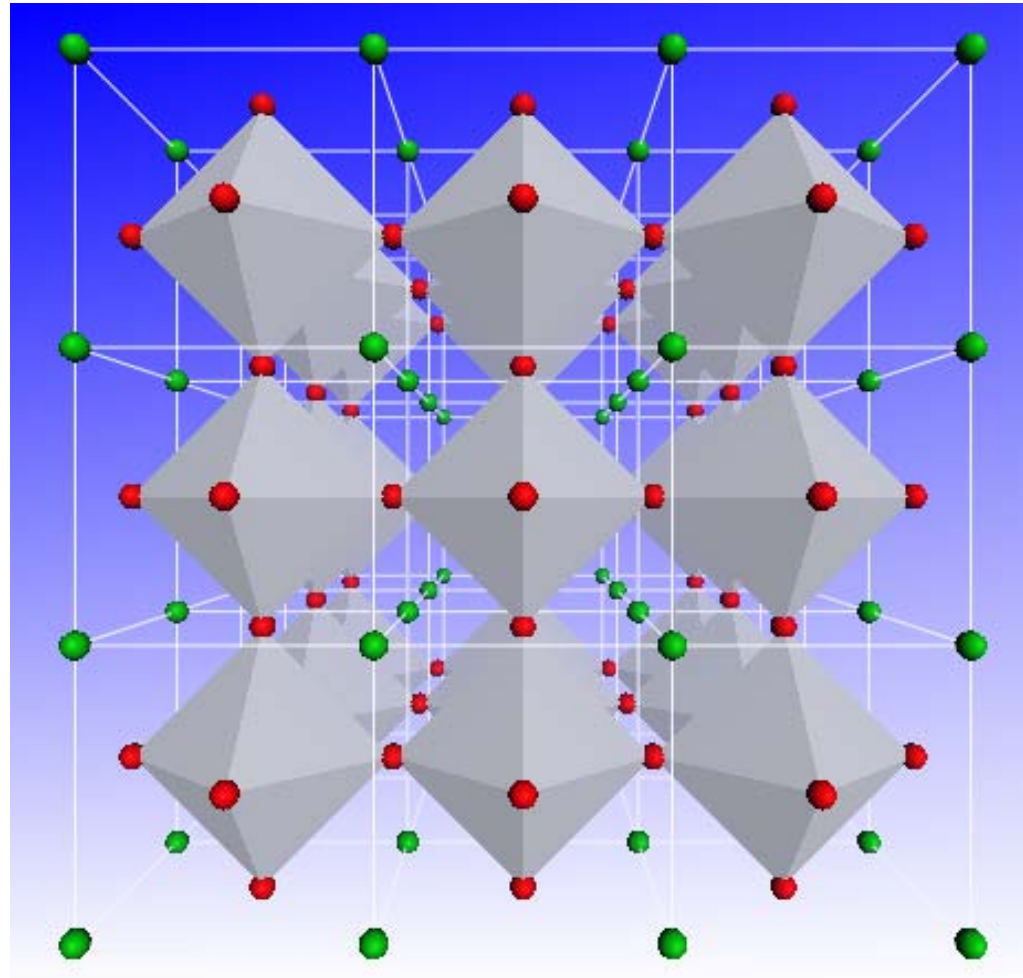
Gramicidin water channel



Water wires within carbon nanotubes

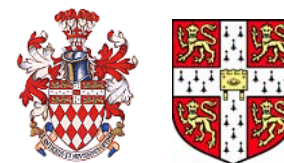


Proton transport through inorganic materials



Outline of programme for first day

- First session (chair: J.A. Elliott) 13:45-15:45
 - Klaus-Dieter Kreuer, MPI Stuttgart
 - Mark E. Tuckerman, New York University
- Discussion and coffee 15:45-16:00
- Second session (chair S.J. Paddison) 16:00-18:00
 - Jacques Rozière, University of Montpellier II
 - Gregory A. Voth, University of Utah
- *Conference photograph* 18:20
 - 6.30pm for 6.30pm: congregate outside Wilson Court
- Dinner and reception in Hall 19:00
 - 7.00pm in Wilson Court for 7.30pm dinner in Hall



Outline of programme for second day

- First session (chair: J.A. Elliott) 09:30-11:30
 - Dr. Gerhard Hummer, NIDDK, Maryland.
 - Prof. Stephen J. Paddison, University of Alabama, Huntsville.
- Coffee & Poster Session 11:30-12:30
- Second session (chair S.J. Paddison) 13:30-15:30
 - Prof. Alexei Kornyshev, Imperial College, London.
 - Dr. M. Saiful Islam, Surrey University, UK.
- Coffee and discussion 15:30-16:00
- Third session (chair S.J. Paddison) 16:00-18:00
 - Prof. Thomas E. DeCoursey, Rush Medical Centre, Illinois.
 - Prof. Robert Slade, Surrey University, UK.
- Informal dinner in town for those staying



Conference Photo

