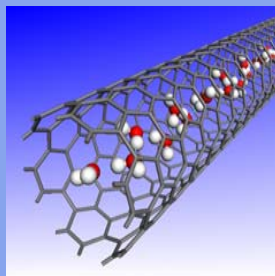
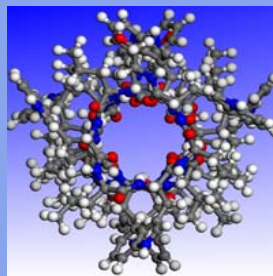
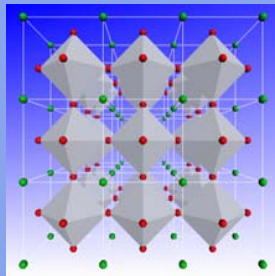
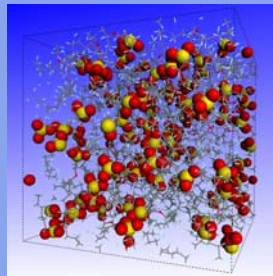


Overview and scope of meeting

11/4/2005

# “Proton conduction in diverse media”

Fitzwilliam College, 11-12th April 2005



James Elliott

Materials Modelling Group

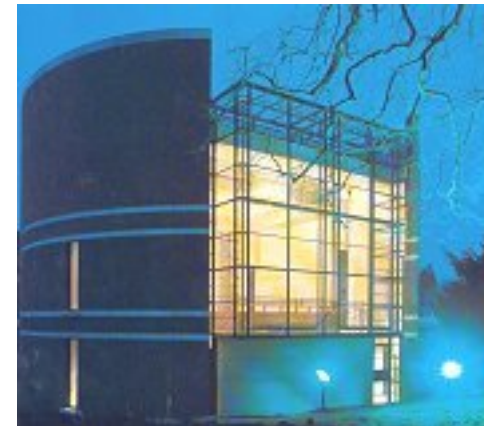
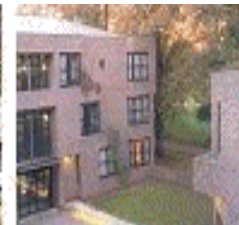
Department of Materials Science & Metallurgy

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>

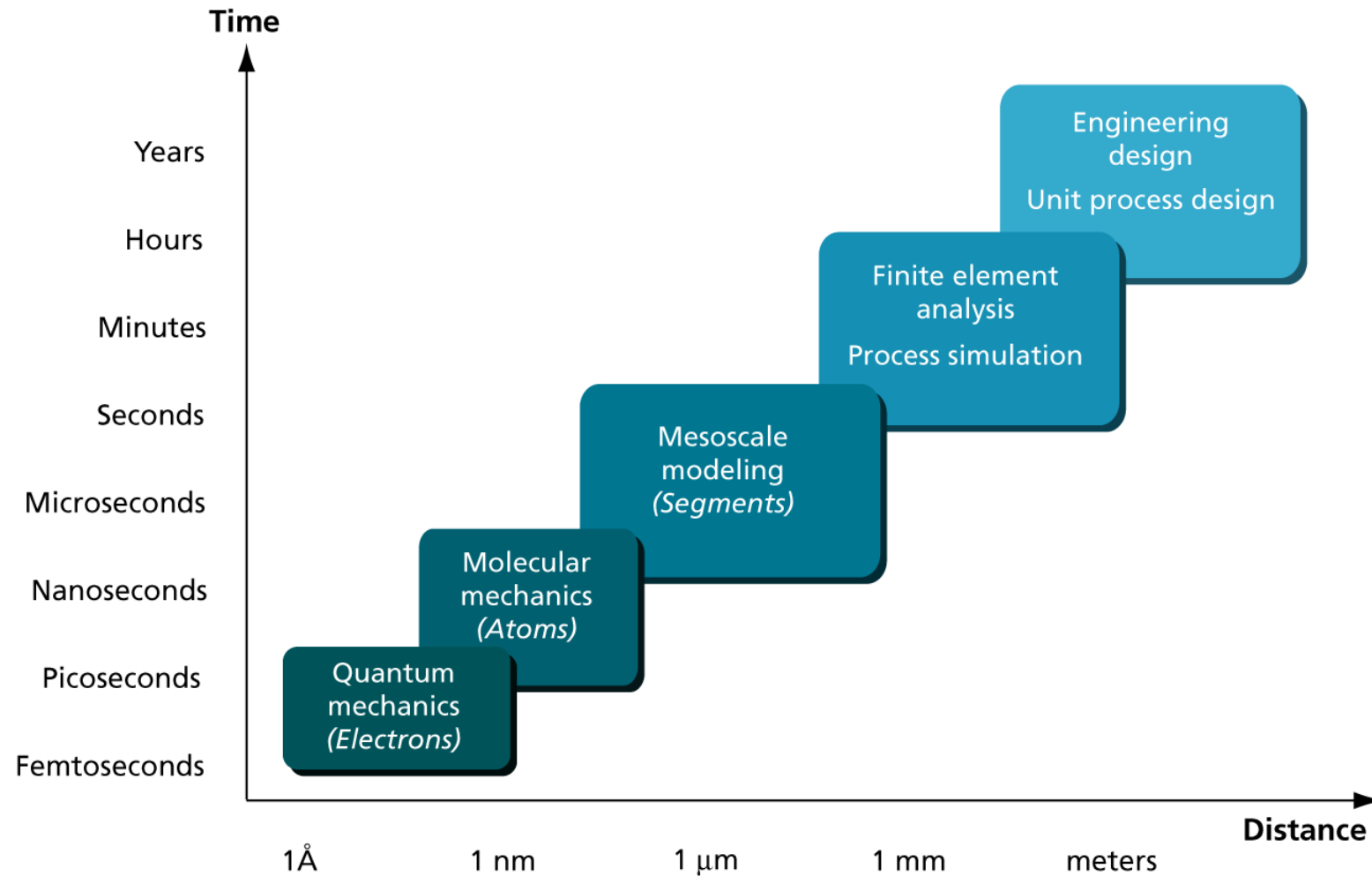


- UK Collaborative Computing Project number 5 (CCP5)  
“... for computer simulation of condensed phases”

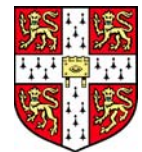
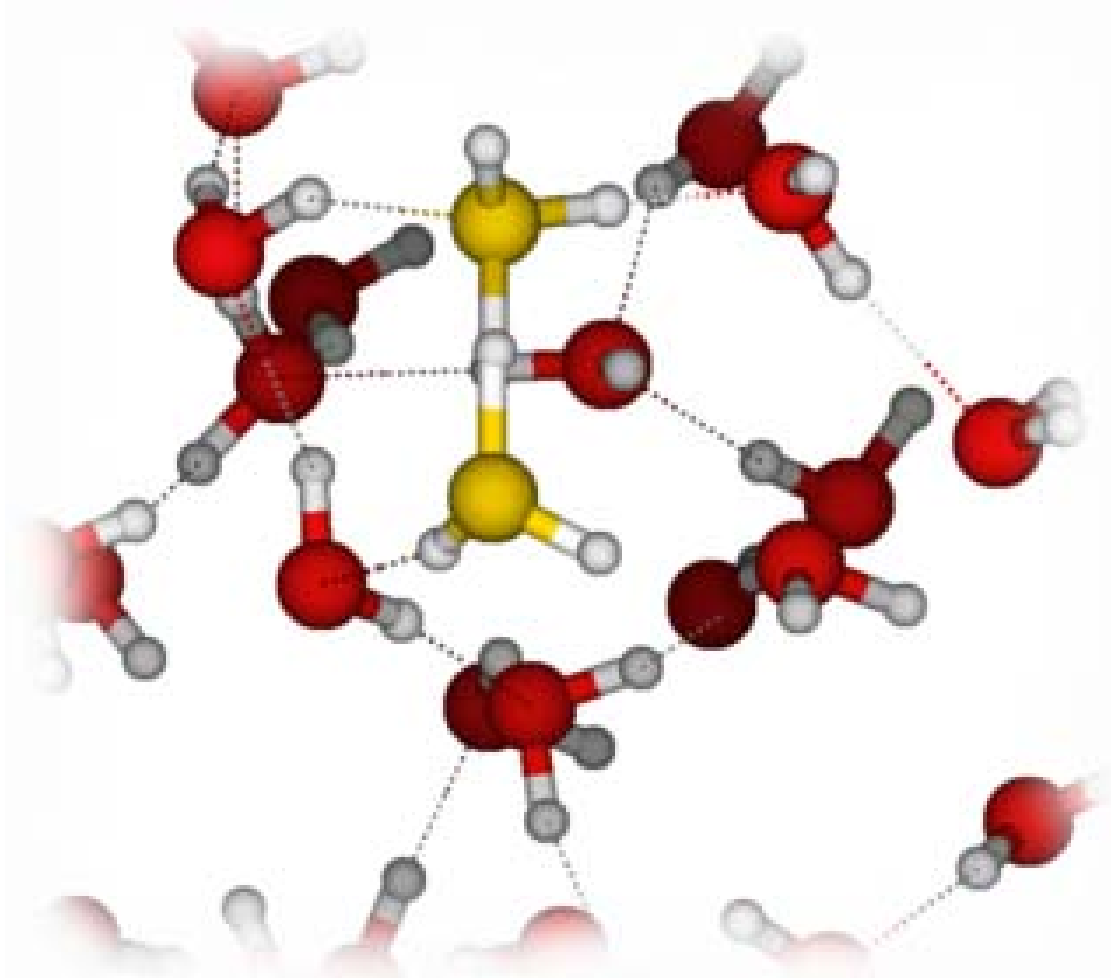
<http://www.ccp5.ac.uk>



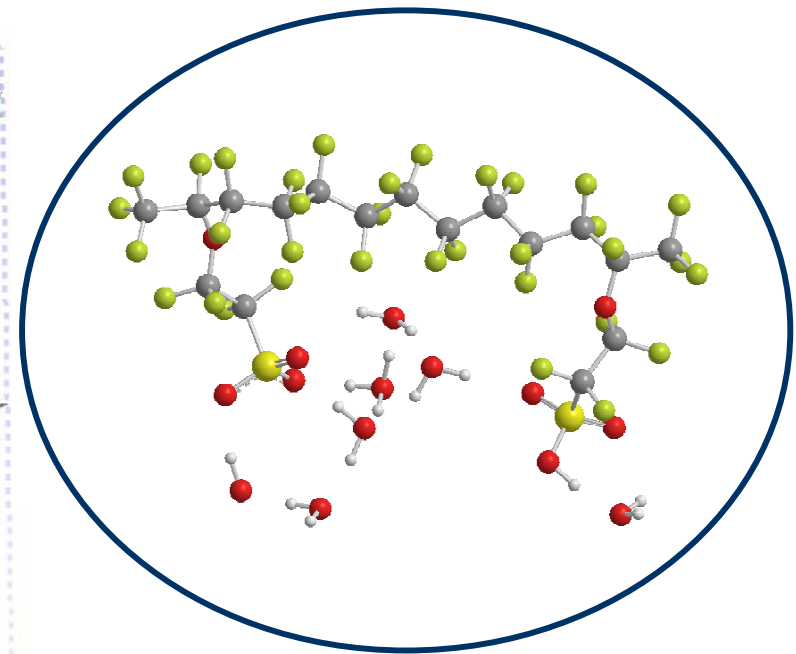
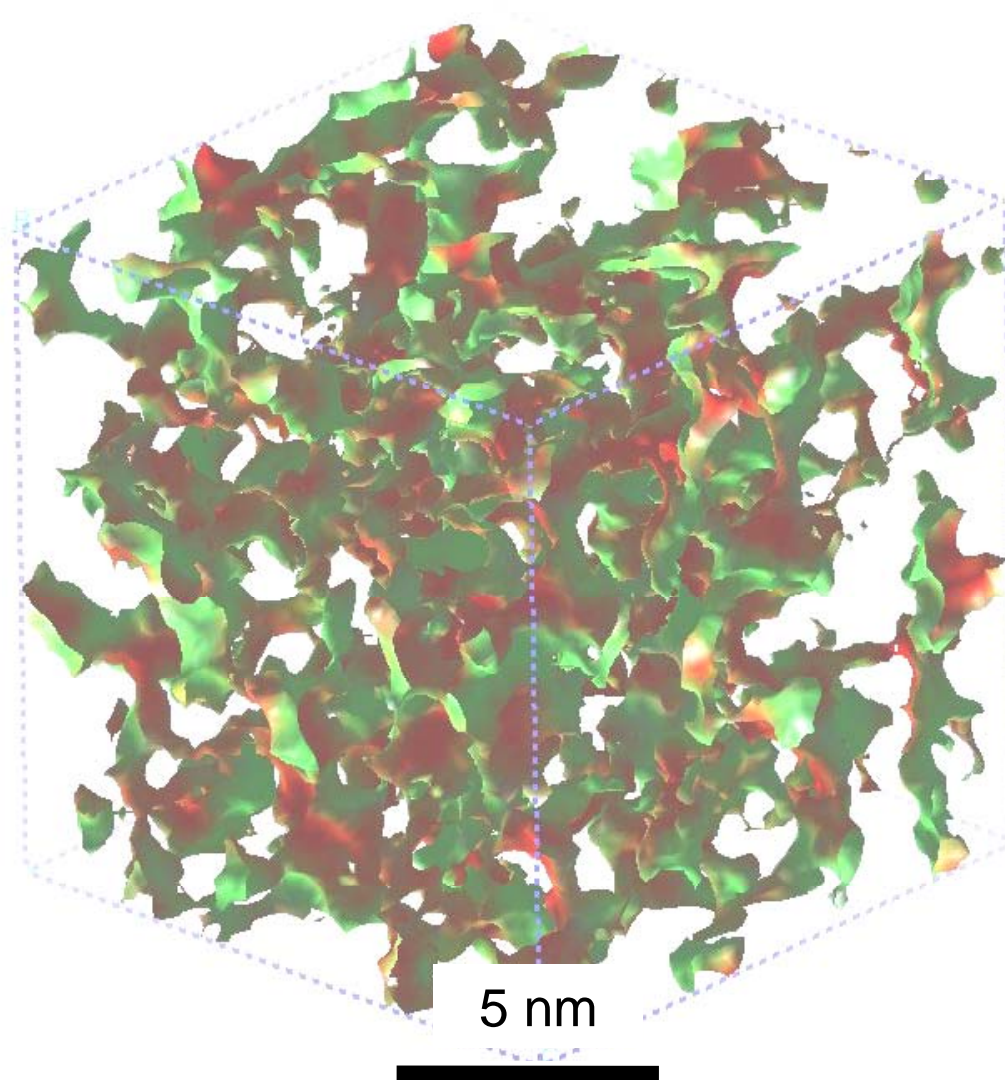
# Multi-scale approach



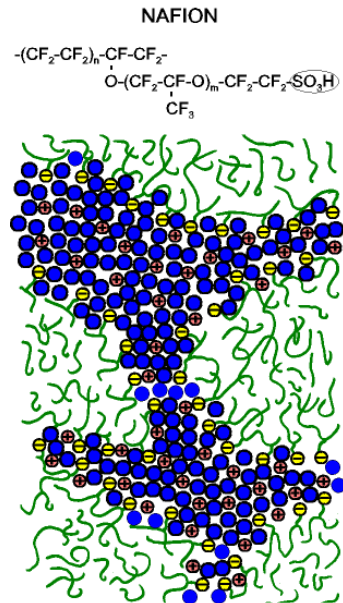
# Proton transport in bulk water



# Polymer electrolyte membranes for fuel cells

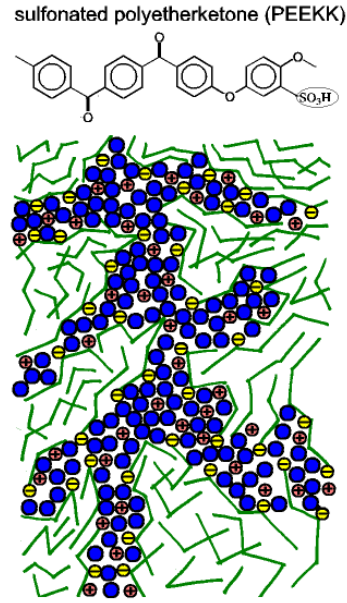


# New membrane materials and composites



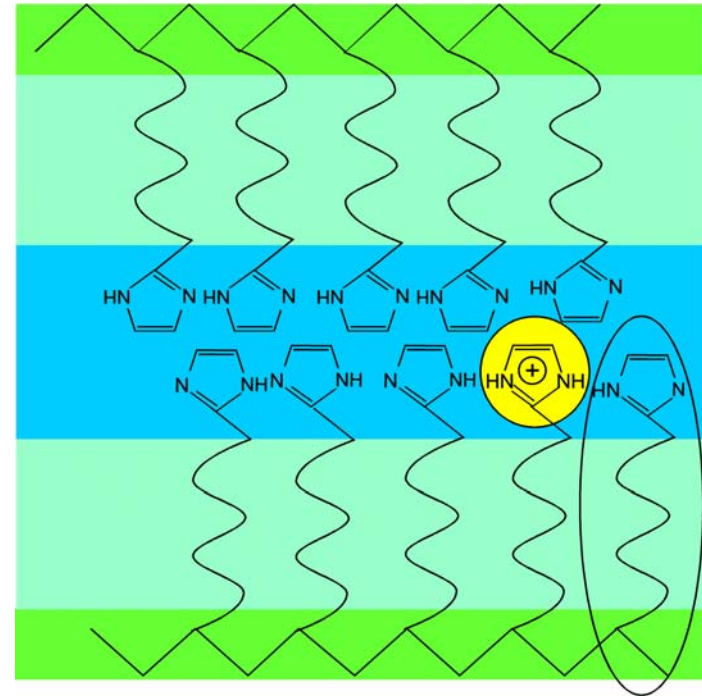
- wide channels
- more separated
- less branched
- good connectivity
- small  $-SO_3^- / -SO_3^-$  separation
- $pK_a \sim -6$

- relevant scales and interactions
- 0,1 nm
  - 1 nm
  - 10 nm



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

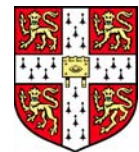
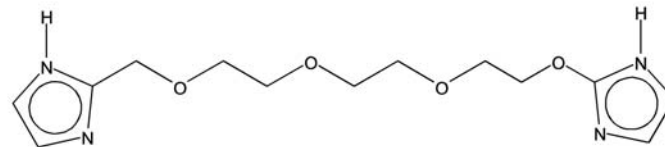
- reactions on molecular scale
- space charge effects (electrostatics)
- percolation



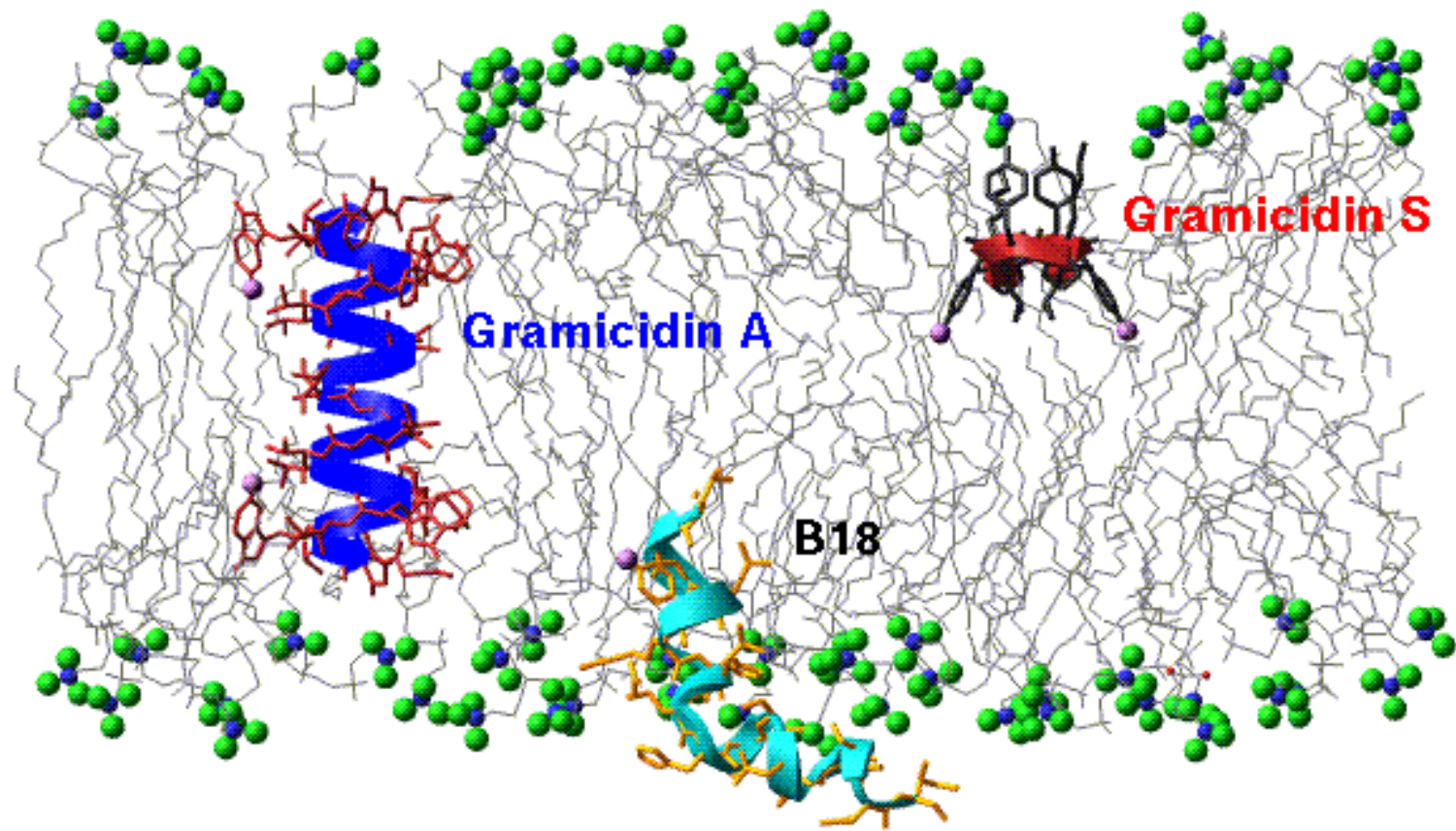
rigid polymer backbone

soft spacer

liquid - like proton solvent

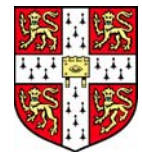
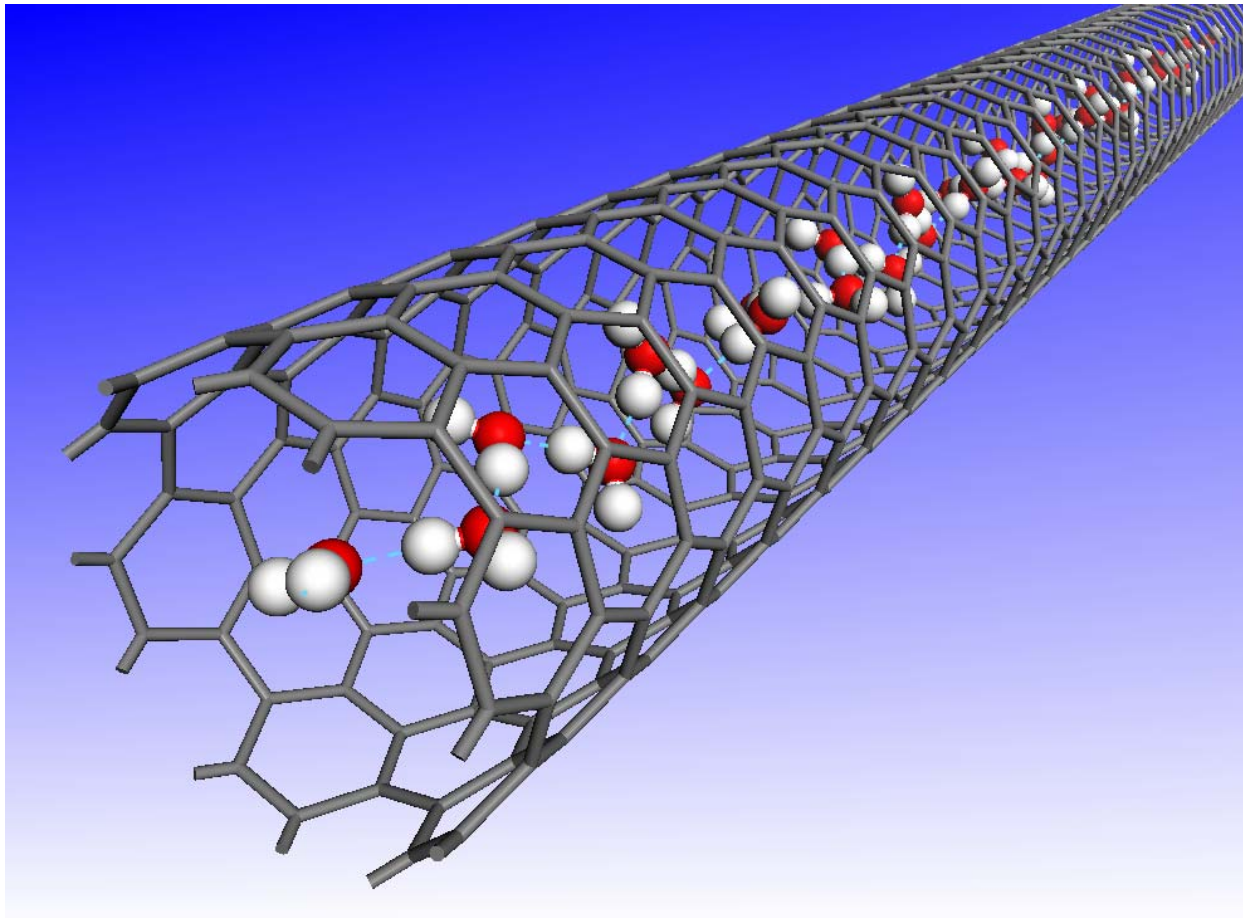


# Gramicidin water channel

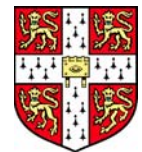
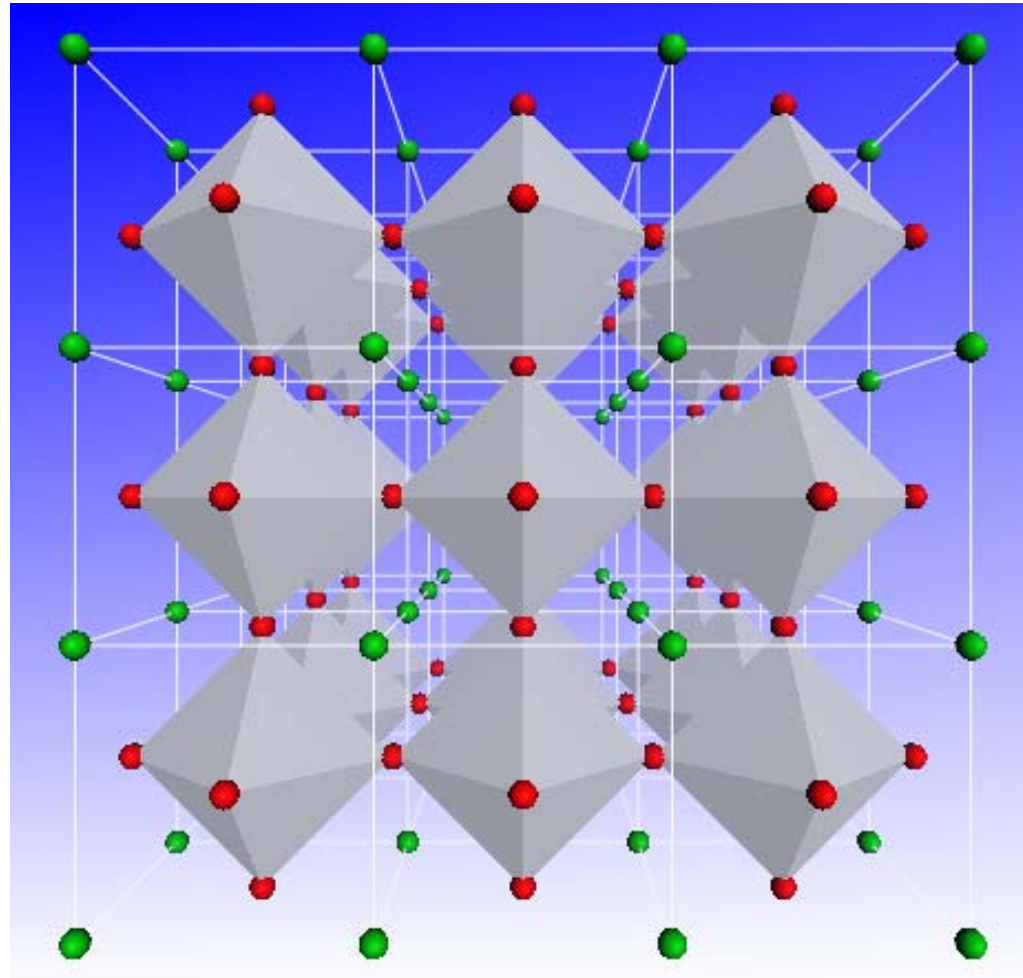




# Water wires within carbon nanotubes

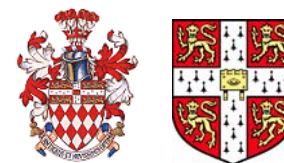


# Proton transport through inorganic materials



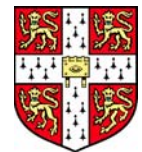
# Outline of programme for first day

- 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

