Dr Philip Wormald

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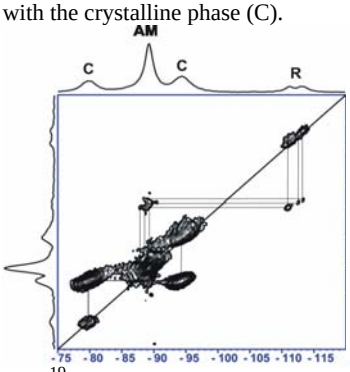
Research Interests:
Development of High and Low field NMR methodologies for the analysis of structure and dynamic processes in polymers and inorganic fluorides.

My research focuses on materials were the specific property of the fluorine nucleus enhances functionality and materials. Our aims are to develop methodologies in NMR spectroscopy and DFT calculations, to gain insight into the structure and physical properties of novel fluoropolymers for advanced material applications i.e. membranes, porous polymers and inorganic fluorides. We are also developing strategies for time domain (TD), diffusion and fast field cycling (FFC) NMR for polymers with tunable properties and morphologies. These projects are in collaboration with research groups in Italy, France, Germany, Canada and the UK.

1) NMR of Fluoropolymers

The combination of homo and hetero nuclear NMR correlation experiments allows us to assign signals in both the ^{19}F and ^{13}C NMR spectra of important novel fluoropolymers synthesised in our labs and in collaboration with partners in France. The Back-to-Back (BABA) experiment allows us to observe spins that are close in space (connectivity). Hence, as seen in below the reverse units (R) of PVDF are in the Amorphous (AM) phase and not associated with the crystalline phase (C).



The structure of PVDF Polyvinylidenefluoride

$-[CH_2CF_2CH_2CF_2]_n-$
Main chain structure

$-[CH_2CF_2CF_2CH_2CH_2\ CF_2]-$
Reverse unit structure

The ^{19}F BABA 2Q-1Q spectrum at 60 kHz MAS of PVDF
This type of experiment allows us to associated signals with macroscopic properties of the polymer i.e. crystallinity, amorphous, reverse unit and end chain content and connectivity. DFT studies are used to confirm spectra

See the group and polymer and NMR centre web sites for postgraduate opportunities.

2) Polymer and NMR centre.

Advanced material applications for Fusion energy research will require well-defined polymers with tunable properties and morphologies. The polymers are modified with varying nuclei and monomers, giving a change in macroscopic properties and structure. We will develop new time domain (TD) NMR methods to monitor changes in situ, during polymerization and the study of diffusion and degree of cross-linking in new very low-density materials

Low field magnetic resonance will be used to probe molecular motion in these polymers. Both Static and fast field cycling (FFC) methods will be developed for this purpose. Principal component analysis (PCA) is used as a tool to correlate all NMR data along with other computational methods. Polymers containing ^{19}F, ^{31}P and large Z nuclei are also under development for a variety of applications.

3) Inorganic fluorides

We are developing multinuclear NMR strategies to decipher the structure of inorganic fluoride systems using ^{19}F fast MAS NMR spectroscopy and 2D applications on quadrupolar and low gamma nuclei i.e. ^{45}Sc and ^{89}Y fluorides. See group page for more information.

SELECTED RECENT PUBLICATIONS

1. Multi-nuclear magnetic resonance and DFT studies of the poly(chlorotrifluoroethylene-altethyl vinyl ether)copolymers. D. Carnevale, P. Wormald*, B. Ameduri and Sharon E. Ashbrook, Macromolecules 2009, 42, 5652–5659.

2. The Direct DIVAM Experiment: A spin Dynamics Analysis. P. Hazendonk*, P. Wormald, T. Montina, ***J. Phys .Chem.*** .**A, 2008**,112 (28) 6262-6274.

3. High-resolution 19F and 1H NMR of a Vinylidene Fluoride Telomer. Wormald P*, B. Ameduri, P. Hazendonk, R.K. Harris. ***Polymer*** 44, 643-651, 2008.

4. Solvothermal synthesis and luminescent properties of two organically-templated chain-structure fluorides, [C4H14N2][MF5] (M = In, Sc), Anil C. A. Jayasundera, Adrian A. Finch, Philip Wormald and Philip Lightfoot. **Chem. Mater**, **2008,** 20, 6810-6815.

5. Fluorine-19 solid-state NMR study of vinylidenefluoride polymers using selective relaxation filters. P. Wormald*, R.K Harris, B. Ameduri. P. Hazendonk, ***Solid State Nucl. Magn. Reson,*** 30 (2006) 114–123.