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Phenylalanine gelation and its dynamics studied through crystal structure analysis.c

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Phenylalanine has been presented as a hydrogelator in a number of papers [1-3]. However, we present our direct measurement of the crystalline properties of these hydrogels and their dynamics as measured by NMR. This data allows for comparison of the gelation in water (known) and in DMSO (our studies). We can nominally describe the Phenylalanine monohydrate crystal structure of the hydrogel as having a hydrophilic two-dimensional layer and a hydrophilic layer that contains the zwitterionic groups and water hydrogen bonded to each other. The dominant electrostatic interactions of the structure inform us of the directionality of crystal growth and potential reasons behind this anisotropic growth of fibres that form the gelation network. With this knowledge in hand, the structures and gel properties are modified, e.g. morphology shown in figure, utilising halogenation of the aromatic group of phenylalanine resulting in further understanding of the gelating properties and correlation to the crystalline phases. The crystal structure analyses reveal how the halogen halogen interactions are competing with the hydrate formation patterns and polarizing the aromatic rings. This provides us with almost unprecedented in-depth details of how Phenylalanine and its derivatives form gels.

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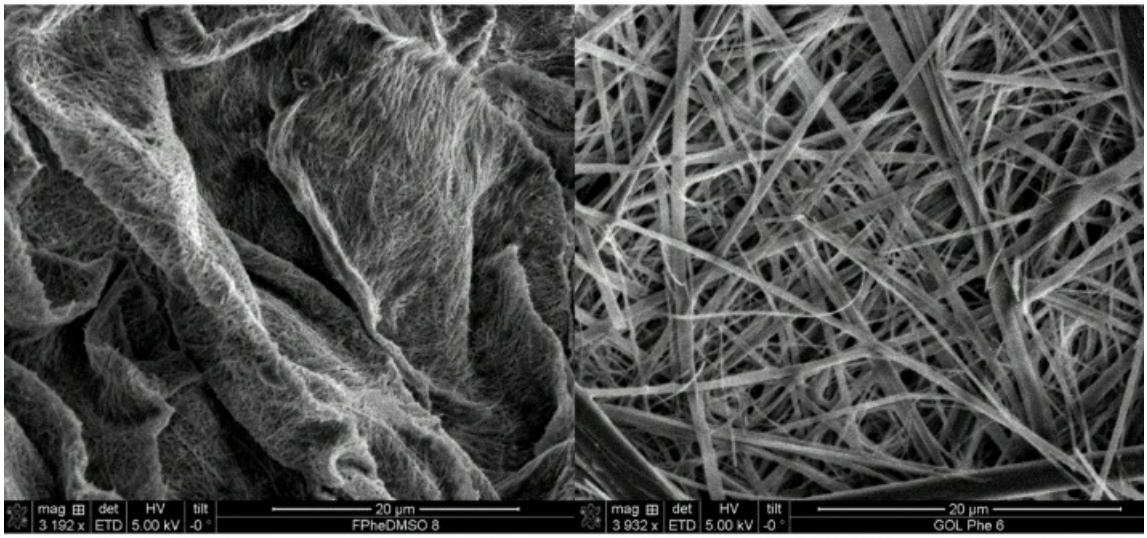

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