

# SOLID STATE NMR STUDY OF CATECHOL BASED POLYMERS

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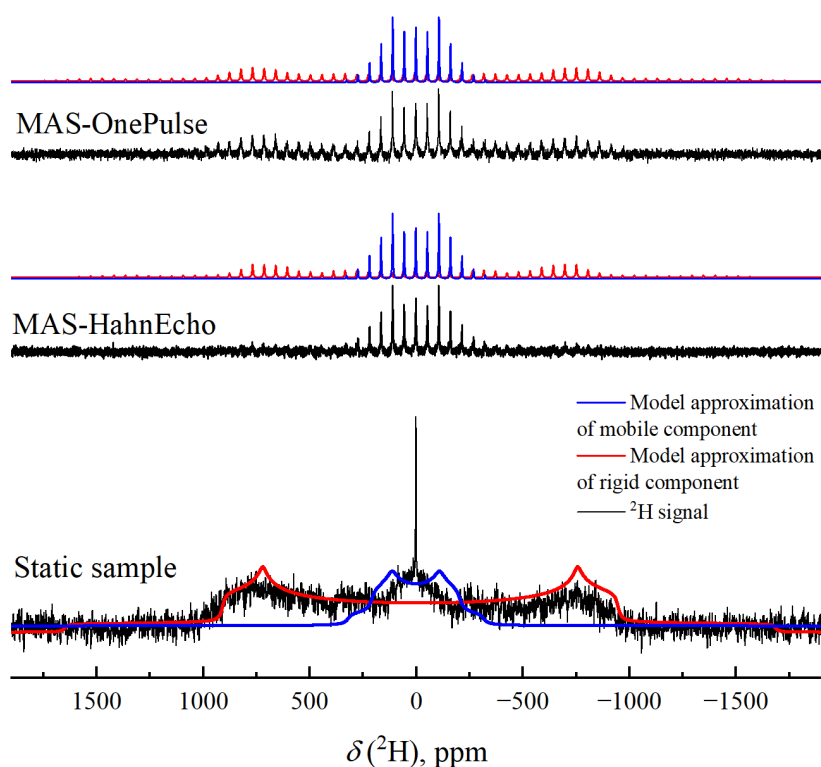
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Bio – mimicking materials containing catechol functional groups that are inspired by the strong adhesion of marine mussels have attracted much scientific attention due to their applications in surface engineering. In this work, the structural properties and molecular dynamics of poly(N-catechol dimethyl acrylamide) (PDMAA) and fumed silica composites (SiO<sub>2</sub>) are investigated using solid-state NMR spectroscopy.

<sup>13</sup>C CP-MAS solid-state NMR spectroscopy confirmed the presence of the polymer in the composites, the <sup>29</sup>Si MAS and CP-MAS led to the conclusion that the adsorption is likely mediated by non-covalent hydrogen bonds rather than covalent bonding,

The specific dynamics of the catechol groups were further investigated using deuterated PDMAA analogs and <sup>2</sup>H MAS NMR spectroscopy at the temperature range from 245 K to 350 K. The quadrupolar line shapes were analyzed using the “DMfit”[1] modeling software, determining the quadrupole interaction constant  $C_Q$  and asymmetry parameter  $\eta$ . The spectral analysis revealed a heterogeneous environment consisting of two distinct configurations of the catechol group: a rigid component with limited mobility, characterized by high  $C_Q$  values, and a more flexible, mobile component. The conducted temperature measurements revealed that the rigid fraction remained stable, while the mobile fraction experienced significant line narrowing due to increased molecular motion (motional averaging).



**Fig. 1.** <sup>2</sup>H NMR and <sup>2</sup>H-MAS NMR spectra of deuterated pure PDMAA(dried), measured at room temperature using different pulse sequences. Blue line indicates the mobile component, the red line indicates the rigid component

Such results provide valuable insights into the complex molecular mobility and ordering of catechol groups in polymer and silica composites.