

Abstract Submitted
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Characterization of the Mobility and Reactivity of Water Molecules on TiO₂ Nanoparticles by ¹H Solid-State Nuclear Magnetic Resonance¹ XIAOLIANG WANG, LILI ZHU, Nanjing University, PINGCHUAN SUN, Nankai University, DONGSHAN ZHOU, GI XUE, Nanjing University — Understanding interfacial water behavior is essential to improving our understanding of the surface chemistry and interfacial properties of nanomaterials. Here using ¹H solid-state nuclear magnetic resonance (¹H SSNMR), we successfully monitored ligand exchange reaction between oleylamine (OLA) and adsorbed water on titanium dioxide nanoparticles (TiO₂ NPs). Three different types of interfacial waters with different reactivities were distinguished. The mobility of the adsorbed water molecules was characterized by dipolar filtered ¹H SSNMR. Our experimental results demonstrate that the adsorbed water can be categorized into three different layers: rigid water species with restricted mobility closest to the surface of TiO₂ NPs; less mobile water species weakly confined on TiO₂ NPs; and water molecules with high mobility. Water in the third layer could be replaced by OLA, while water in the first and second layers remained intact. The finding that the interfacial water with the highest mobility has the strongest reactivity has guiding significance for tailoring the hydrophilic and hydrophobic properties of TiO₂ NPs.

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