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Real-space imaging of interfacial water with submolecular resolution[1] YING JIANG, International Center for Quantum Materials (ICQM) and School of Physics, Peking University, PEKING UNIVERSITY TEAM — Water/solid interfaces are vital to our daily lives and also a central theme across an incredibly wide range of scientific disciplines. Resolving the internal structure, i.e. the O-H directionality, of water molecules adsorbed on solid surfaces has been one of the key issues of water science yet remains challenging. Using a low-temperature scanning tunneling microscope (STM), we report the submolecular-resolution imaging of individual water monomers and tetramers on NaCl(001) films supported by a Au(111) substrate at 5 K. The frontier molecular orbitals of adsorbed water were directly visualized, which allowed discriminating the orientation of the monomers and the H-bond directionality of the tetramers in real space. Comparison with ab initio density functional theory calculations reveals that the ability to access the orbital structures of water stems from the electronic decoupling effect provided by the NaCl films and the precisely tunable tip-water coupling.

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