

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Real space imaging of buckled tetramer and flat hexamer water cluster on Au(111) surface: determine structures of water clusters on solid surface¹ ANNING DONG, LEI YAN, LIHUAN SUN, XINYAN SHAN, YANG GUO, SHENG MENG, XINGHUA LU, Institute of Physics, Chinese Academy of Sciences, SF05 TEAM, SF10 TEAM — The configuration of hydrogen bond network in water clusters is important but there still exist debates. For example, a flat configuration of water hexamer has been observed by scanning tunneling microscope (STM), whereas a buckled configuration is favored in density functional theory (DFT) simulation. One of the difficulties in solving such puzzle is due to the lack of high-resolution images and controlled cluster reconstruction, especially for water clusters consists of no more than 6 water molecules. Here we present low-temperature STM images of water clusters with unprecedented spatial resolution which clearly reveal precise configurations of isolated water clusters on Au(111) surface. While water tetramers present a buckled configuration, water hexamers all features a flat configuration, in which the apparent height of each water molecule is the same as the height of the two low-lying molecules in the buckled tetramer. Transformations from a flat hexamer to buckled tetramer and pentamer are achieved by molecule manipulations, which illustrates the competition between hydrogen bond interactions and van der Waals interactions. With combined DFT calculations, the features of hydrogen bond network and van der Waals interactions in such a system are further determined.

¹National Science Foundation of China under grant no. 11174347, 61027011, and 61376100.

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Date submitted: 08 Nov 2016

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