Element-dependent growth of metal clusters on the 2D metal organic framework

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Two-dimensional metal-organic frameworks (2D-MOFs) are formed by co-adsorption of metal atoms and organic molecules on various solid surfaces such as Cu. Adsorption of 1,3,5-tris(4-bromophenyl)benzene (TBB) molecules on Ag(111) and subsequent heating of the substrate result in the porous 2D-MOF shown in Fig. 1. By deposition of metal atoms onto the 2D-MOF, metal nano-clusters are obtained, and the 2D-MOF plays a role of a template to grow the metal clusters in the pores [1,2].

In this study, Ag, In, and Pd atoms are deposited on Ag(111) with the 2D-MOF, and we found that the different growth phenomena for Ag, In, and Pd clusters by scanning tunneling microscopy (STM) measurements [3]. Ag clusters are grown on the 2D-MOF, and In clusters are grown in the pore of the 2D-MOF. On the other hand, Pd clusters are grown at the unconnected terminals of the 2D-MOF. In addition, the deposited Pd atoms sometimes break the 2D-MOF, and Pd clusters are also grown from the broken positions of the 2D-MOF.

We calculated the energy of the Ag, In, and Pd adatom at the pore of the 2D-MOF as a function of the distance from the 2D-MOF (the center of the pore is the furthest position) by density functional theory (DFT) calculation. Ag and Pd adatoms in a pore have lower energies closer to the 2D-MOF, and In adatom has higher energy closer to the 2D-MOF. It indicates that the interaction of Ag and Pd adatoms with the 2D-MOF are attractive and that of an In adatom is repulsive. The details of the interactions and the growth mechanisms will be discussed in the presentation.

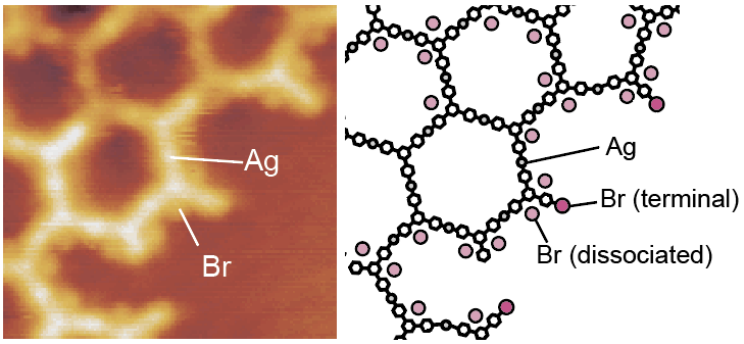

Fig. 1. An STM image of the 2D-MOF on Ag(111) and the schematic drawing of the 2D-MOF.

[1] M. Pivetta et al., Phys. Rev. Lett. **110**, 086102 (2013).
[2] R. Zhang et al., ACS nano, **9**, 8547 (2015).
[3] N. Tsukahara et al., Langmuir, to be submitted.