

CONFINEMENT OF A MOLECULE IN A MOLECULAR FENCE STRUCTURE ON SILICON SURFACE

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As an alternative nanoelectronics technology to photolithography, single-molecular electronic devices have received major attention. In such devices, each single molecule that has an electronic function, such as a resistor, condenser, and transistor, is fixed in between metallic electrodes. However, inserting a specific molecule between the electrodes and connecting the molecule with the electrodes firmly are the processes need to be overcome for fabrication as a mass product. In this study, we propose a different approach to the single molecular device utilizing a motion of a molecule. Attachment of molecule on a semiconductor surface can change electronic states of the surface drastically. We confined trimethylphosphine (TMP) in a molecular fence structure with a diameter of 1 nm. The movement of TMP was observed by scanning tunneling microscopy (STM).

The molecular-fence structure was formed by an exposure of the clean Si(111)-(7x7) surface to pyrrole molecules at room temperature. Because pyrrole tends to adsorb only on center adatom of the surface, the honeycomb-shaped molecular fence structure is formed self-assembly. After formation of the molecular fence structure, the sample was exposed to TMP gas. Then, the surface was observed by STM in atomic resolution. It was found that TMP adsorbed inside of the molecular fence structure. We also studied dynamic behavior of the molecules with continuous STM scans. During STM scans, the molecular fence structure was stable without chemical bonds cleavage. On the other hand, TMP molecule was moved frequently inside of the molecular fence structure with cleavage of a bond between phosphorous atom of TMP and an adatom of the Si surface.

We also studied the behavior of TMP and pyrrole theoretically. We performed density functional theory (DFT) calculations using Gaussian 09 code. The calculation results indicate that adsorption of two TMP molecules in a half-unit cell of the 7x7 surface is more unstable than adsorption of two TMP in different half unit cells. It suggests that there is a repulsive interaction between TMP molecules attached on the surface.