

Photoemission investigation of 1,5-Cyclooctadiene and Cyclooctene on the Si(100)2×1 surface

M. Kim, J.Y. Baik, C. Jeon, B. So, H.-N. Hwang*, C.C. Hwang*, C.-Y. Park

Department of Physics, BK21 Physics Research Division and Center for Nanotubes and Nanostructured Composites (CNNC), SungKyunKwan University,

*Beamline Research Division, Pohang Accelerator Laboratory (PAL), POSTECH

The 1,5-Cyclooctadiene (COD) and Cyclooctene (COE) on the Si(100)2×1 surface were investigated using C 1s core-level photoemission spectroscopy at Pohang Accelerator Laboratory (PAL). The reaction of COD on Si(100)2×1 surface is termed as a [2+2] cycloaddition, one (or two) C=C double bond of COD reacts with a silicon dimer(s) and forms a Si₂C₂ four-membered ring (di-σ bonds). Up to now, two conflicting structures of COD were suggested: the upright model proposed from the empirical results and the bridge model suggested from a theoretical calculation. To clarify the structure of COD on the Si(100) surface, the C 1s spectra of COD were compared with those of COE. The C 1s spectra of COD on the Si(100)2×1 surface at room temperature were found to consist of two components with binding energies of 283.9 and 284.6 eV, which can be ascribed safely to Si-C and C-C (and/or C=C) bonds, respectively. Interestingly, it was found that the C 1s spectrum of COE has nearly the same line shape with COD at saturation coverage. COE is expected to form an upright structure because it has a C=C bond. Thus, the similarity of the C 1s spectra suggests that COD may prefer the upright structure rather than the bridge structure. This implicates that COD on the Si(100)2×1 surface leaves an unsaturated C=C bond toward the vacuum side which could be used to further reactions with functional molecules.