A-13

실리콘표면에서 화학흡착에대한 메커니즘 연구

Mechanistic study of chemical adsorption on silicon surface

이희순*,**,†, 장현주***, 최철호**

*한국화학연구원, **경북대학교 화학과, ***한국화학연구원,나노물성

(hslee@krict re kr†)

Surface chemistry on semiconductor surfaces has gained enormous popularity recently and the interest is still growing This may be partially due to the tremendous potential of the new functionalities of synthetically modified surfaces Furthermore, the well-ordered silicon surface, especially Si(100)-2x1, provides a unique environment in which a great deal of existing chemical knowledge can be tested Multi-reference wavefunctions in combination with QM/MM were used to study the ethylene and 2-butene surface reactions on Si(100) in their lowest energy singlet states In addition to the diradical pathway, a π-complex pathway on the ethylene surface was found

A significantly different reaction channel is found in the 2-butene surface reaction on Si(100), in which a methyl hydrogen easily transfers to the surface yielding a new type of surface product other than the expected [2+2] cycloaddition product, with a comparatively small activation barrier

The adsorption mechanisms of organic molecules on the Si(100) surface will be discussed