SST-003

Chemical Understanding of Surface Reactions

최철호[1]

[1]경북대학교 자연과학대학 화학과

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. It is conceivable that, as the size of electronic devices based on crystalline silicon wafers shrinks, the surface characteristics of semiconductor materials become crucial for the proper functioning of devices. With the help of traditional organic and organometallic chemistry, a wide variety of new chemically modified silicon surfaces can be synthesized to provide fine tailoring of surface characteristics for a broad range of applications. In addition, to gain the control needed to fabricate an organic function into existing semiconductor technologies and ultimately to make new molecule-scale devices, a detailed understanding of the adsorbate surface as well as interfacial chemical reactions and their products at the atomic/molecular level is critical. To accomplish this, both novel experiments and theoretical investigations need to play a significant role in the advance of this field. This talk begins with the chemical methodologies adapted for surface studies and then proceeds to a consideration of the unique features of clean silicon surfaces. Then, the main focus is directed to the structures and reaction mechanisms of organic molecules on silicon surfaces.

SST-004

Electronic Structures and Bonding Characteristics of Hydrogen Adsorbed on Ethylene Oxides: Toward A Room-Temperature Hydrogen Storage System

Young-Kyun Kwon

Department of Physics and Research Institute for Basic Sciences, Kyung Hee University

Using ab initio density functional theory, we have found that molecular hydrogen binds with oxygen atoms in oligomers of ethylene oxide optimally for hydrogen storage. Through the orbital analysis, we present the special binding mechanism that enhances the binding between a hydrogen molecule and the oxygen atom in ethylene oxide by electron donation and back-donation. Our theoretical model and molecular dynamics simulations also predict that adsorption-desorption process of molecular hydrogen on ethylene oxide can occur in ambient conditions, $T \sim 300$ K and $P = 1$ - 13 atm, achieving gravimetric storage capacity of hydrogen up to 6.2 wt %.