【SP-05】

Theoretical Study of Cycloaddition Reactions of C_2N_2 on the Si(100)-2×1 surface

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In previous study for thermal decomposition of C_2N_2 on Si(100) 2 × 1 and Si (111) 7 X 7 using TPD, XPS, UPS, and HREELS, Lin et al. reported that chemiadsorbate product with nitrile group and mixture of silicon carbide and silicon nitride was formed at various temperature. But detailed possible surface mechanism and structure of products was not described. Thus, we performed a kinetic study on the cycloaddition of C_2N_2 and Si(100) 2 × 1 in order to investigate its chemical properties and reactivity. QM/MM(quantum mechanics/ molecular mechanics), DFT, CASSCF(complete active space-SCF), and MRMP2 methods were used to estimate surface adsorption reaction bearing strong radical character. As a results, we predicted a (2+2)cycloaddition product and isomerized product with nitrile group. We will report the structures of transition states, intermediates and reactivity along the reaction coordinate.