Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

**Adsorption of CO Molecules on Si(001) at Room Temperature**
EONMI SEO, Korea University of Science & Technology, Korea Research Institute of Standards and Science, DAEJIN EOM, Korea Research Institute of Standards and Science, HANCHUL KIM, Department of Physics, Sookmyung Women's University, Korea, JA-YONG KOO, Korea University of Science & Technology, Korea Research Institute of Standards and Science — Initial adsorption of CO molecules on Si(001) is investigated by using room-temperature (RT) scanning tunneling microscopy (STM) and density functional theory calculations. Theoretical calculations show that only one adsorption configuration of terminal-bond CO (T-CO) is stable and that the bridge-bond CO is unstable. All the abundantly observed STM features due to CO adsorption can be identified as differently configured T-COs. The initial sticking probability of CO molecules on Si(001) at RT is estimated to be as small as $\sim$ 1 x $10^{-4}$ monolayer/Langmuir, which is significantly increased at high-temperature adsorption experiments implying a finite activation barrier for adsorption. Thermal annealing at 900 K for 5 min results in the dissociation of the adsorbed CO molecules with the probability of 60-70% instead of desorption, indicating both a strong chemisorption state and an activated dissociation process. The unique adsorption state with a large binding energy, a tiny sticking probability, and a finite adsorption barrier is in stark contrast with the previous low-temperature (below 100 K) observations of a weak binding, a high sticking probability, and a barrierless adsorption. We speculate that the low-temperature results might be a signature of a physisorption state in the condensed phase.

Eonmi Seo
Korea University of Science & Technology,
Korea Research Institute of Standards and Science

Date submitted: 11 Nov 2014 Electronic form version 1.4