The 56th ICYS Special Seminar

Dr. Binghai Yan

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Title: Electronic and structural properties of the Ge(001) surfaces with impurity dimers: first-principles study (Chair: Dr. Canhua Liu)

Recently, an atomic switch is fabricated using STM by Tomatsu et al. (Science 315 (2007) 1696) by the conduction of the 1D surface state using the buckled Sn-Ge dimer on Ge(001). Collaborated with Tomatsu et al., we investigated the electronic properties of Ge(001) and the ON/OFF mechanism of the atomic switch. Using the first-principles method, we calculated the scattering potentials induced by different impurity dimers and obtained good agreement with STM phase shift measurements. We further studied the switch mechanism related with dimer flip motion by electron injection from STM tip. We propose that the flip motion is caused by a resonant scattering of the π* electrons with localized electronic states.

References: [2] K. Tomatsu, B. Yan et al. Phys. Rev. B 78, 081401(R) (2008). [1] K. Tomatsu, B. Yan, et al. Surf. Sci. 603, 781 (2009). [3] B. Yan et al., Phys. Rev. Lett. 103, 189701 (2009) [4] B. Yan, K. Tomatsu et al., Phys. Rev. B, B 79, 235437 (2009)

Venue: **Seminar Room #431, MANA Bldg.,**

Date: **November 25th Wednesday** ***Time:*** **15:30-16:15**

NAMIKI Site

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