# 776th ASRC Seminar

**Date**: 令和2年1月15日(水) 11:00 ～

**Location**: 第1センター会議室(103会議室)

**Speaker**: Prof. Ludo B. F. Juurlink
(Leiden University, The Netherlands)

**Title:** The dynamical origins of defect-controlled surface reactions


要旨: **Reactive collisions of $H_2$ and $O_2$ molecules with the surface of catalytic particles are central to many heterogeneously (electro)catalyzed reactions. They also serve as model systems to develop improved theoretical methods for predicting chemical reaction dynamics and kinetics. It is well established that atomic-level corrugation often, but not always, increases reactivity toward both molecules.**

**To unveil the dynamical origin of this behavior, we have developed a curved single surface approach. The curved surface of c-Pt(111)[11-2]31° single crystal provides a continuous variation over 3 orders of magnitude in monoatomic step density with spatial separation of two common step types. In combination with spatially-resolved supersonic molecular beam techniques, we unravel to what extent and how monoatomic steps control single collision events. For $O_2$, dissociation is predominantly indirect. At low collision energies, sticking scales linearly with step density. With dr. Kurahashi (Tsukuba, Japan), additional state-selected and rotationally aligned $O_2$ experiments resolve that monoatomic steps provide geometric corrugation allowing for efficient trapping into the physisorbed state preceding dissociation. For higher energies, we identify direct access to various chemisorbed states. For $H_2$, our results show that the dissociation mechanisms are – on the contrary - direct and elementary, resolving a 40-year old debate. We have also used a second curved Pt crystal with a rotated azimuthal direction to resolve how kinks in step edges affect the collision. We determine absolute reaction cross sections for parallel dissociative mechanisms at various defect sites.**



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