



## グローバル COE 物質科学イノベーション講演会

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演 題：

# On the role of hydrogen in heterogeneously catalyzed reactions

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日 時：2010年7月5日（月）16:00-17:30

場 所：創成科学研究棟4F セミナー室 B (04-214)

要 旨： Hydrogen is a frequent participant in several heterogeneously catalyzed reactions, including Fischer-Tropsch Synthesis (FTS) of fuels, ammonia synthesis, oxygen reduction reaction (ORR), NO reduction, preferential oxidation of CO in the presence of H<sub>2</sub> (PROX), etc. Having analyzed the detailed aspects of the reaction mechanism for a number of these reactions on various transition metal and alloy surfaces using first-principles methods, some common principles governing the role of hydrogen in a wide range of catalytic transformations begin to emerge. In this presentation, we will discuss these common mechanistic principles by examples, including FTS, ORR, PROX, through an analysis of the energetics of alternative elementary reaction steps and the resulting potential energy diagrams. Connections to observations from experimental studies provide an invaluable perspective for the evaluation of our theoretical assessments.

### REFERENCES

"Structure sensitivity of methanol electrooxidation on transition metals", *JACS*. (2009).

"Modeling ethanol decomposition on transition metals: a combined application of scaling and Bronsted-Evans-Polanyi relations", *JACS* (2009).

"Ru-Pt core-shell nanoparticles for preferential oxidation of carbon monoxide in hydrogen", *Nature Materials*, (2008)

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