東京大学グローバルCOEプログラム　機械システム・イノベーション国際拠点

東京大学 THE UNIVERSITY OF TOKYO

GMSI Global Center of Excellence for Mechanical Systems Innovation

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## Complexity and emergent behavior in catalytic reactions: CO oxidation on gold and ammonia decomposition on single metals and bimetallics


## Professor Dionisios G. Vlachos

**Elizabeth Inez Kelley Professor of Chemical Engineering**
**Director of Catalysis Center for Energy Innovation**
**University of Delaware, Newark, DE 19716-3110, U.S.A.**


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## 要旨


In this talk, complexity and emergent behavior of catalytic reactions will be presented with main focus on discovery of novel catalytic materials. In particular, the effects of support, and particle size and shape will be addressed. Two prototype reactions will be discussed: CO oxidation on Au supported on MgO and ammonia decomposition for hydrogen Production. Phenomenal structure sensitivity of ammonia is found experimentally by combining EXAFS, TEM, chemisorption, and reactivity data. In particular we show that not only size but also particle shape can affect activity dramatically. Multiscale modeling is in excellent agreement with data. We then formulate an optimization problem to predict best catalytic bimetallic materials that we subsequently design and demonstrate experimentally. We use multiscale modeling, combining density functional theory with kinetic Monte Carlo simulations, to understand the overall activity of CO on Au particles and small clusters. We find that oxygen Vacancies are critical in enabling charge transfer and thus molecular oxygen adsorption. Carbonate poisoning and catalyst restructuring are key processes in understanding activity of Au clusters.



主催：　東京大学グローバルCOEプログラム「機械システム・イノベーション国際拠点」
本件連絡先：　東京大学大学院工学系研究科化学システム工学専攻　教授　大久保達也
E-mail: okubo@chemsys.t.u-tokyo.ac.jp　Phone: 03-5841-7348
GCOE事務局　E-mail: gmsi-office@mechasys.jp　Phone: 03-5841-7437