Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Precious metal-free catalyst for purification of automotive exhausts: NO dissociation on Cu oxide surfaces KUNIYUKI MIWA, Department of Applied Physics, Osaka University, HIDEAKI KASAI, Department of Applied Physics, Osaka University; Center for Atomic and Molecular Technologies, Osaka University, ALLAN ABRAHAM PADAMA, JOAQUIN LORENZO MORENO, Department of Applied Physics, Osaka University — The dissociation of NO_x molecule on catalysts is the rate-limiting step for its reduction process and is the subject of recent investigations related to exhaust gas purification. Three-way catalysts which are composed of Rh, Pd and Pt, are known to work well for such purpose; however, their expensive cost hinders their applicability. In this work, Computational Materials Design based on density functional theory was employed to test the efficiency of Cu-based catalysts for NO dissociation. It was found that the dissociation path of NO on Cu-terminated $Cu_2O(111)$ and CuO(110) surfaces is comparable with Rh(111). This is attributed to the modified electronic structure of the surface Cu atoms of Cu oxides in comparison with Cu(111). The calculated NO dissociation barriers are lower and the binding energies of co-adsorbed N and O atoms are weaker on Cu oxides than on Rh(111), which is favorable for subsequent reactions. Our experimental collaborator had also verified that Cu oxides can be better catalysts than Rh, Pd and Pt for the purification of exhaust gases. The details of this work and the oxidation of CO in the presence of dissociated NO will be discussed in the meeting.

Hideaki Kasai
Department of Applied Physics, Osaka University; Center for Atomic and Molecular Technologies, Osaka University

Date submitted: 21 Dec 2013 Electronic form version 1.4