Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

First-principles analysis of vacancy-assisted reaction on metal-doped t-ZrO_2 surfaces[1] SANTANU CHAUDHURI, HYUNWOOK KWAK, Washington State University — Vacancy-assisted reaction on tetragonal (t-) ZrO_2 surface is important for its potential in combustion synthesis, barrier coating and as solid electrolyte in solid-oxide fuel cells. Doping or alloying the surface could significantly enhance the surface reactivity and transport by altering the electronic structure of the surface. We performed first-principles analysis on the metal doped t-ZrO_2 surfaces to assess the role of metal doping on the vacancy-assisted reaction at t-ZrO_2. Vacancy formation energy was calculated for 14 different doping metals. Most impurity metals from 4th and 5th row of periodic table promote formation of vacancies on the surface. Electronic structure of the defect state with respect to filled states and vacancy diffusion barriers will be discussed. Furthermore, the analysis is extended to surface reactivity for oxygen adsorption during combustion reaction of Zr particles and barrier properties against water mediated corrosion processes. For both cases, an analysis of reaction rates under different temperatures and pressures for different t-ZrO_2 surfaces will be discussed.

[1]This work has been supported in part by DARPA grant W911NF-09-C-0033 and ONR grants N00014-04-1-0688 and N00014-06-1-0315.

Hyunwook Kwak
Washington State University

Date submitted: 18 Nov 2009 Electronic form version 1.4