



BNL-101131-2013-CP

Utilizing interfaces: One-step forward for rational design of heterogeneous catalysts

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*Internal Seminar
ExxonMobil Research and Engineering Company
Corporate Strategic Research
Clinton, NJ
June 20, 2013*

June 2013

**Center for Functional Nanomaterials
Brookhaven National Laboratory
U.S. Department of Energy
Office of Science**

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As far as heterogeneous catalysts are a composite material, physicochemical properties of the interfaces between individual components should be extensively studied for rational design of catalysts with desired properties.

Here, I will present recent *computational achievements* in following three heterogeneous catalysts where the interface between composing materials plays a critical role:

- 1) CO oxidation by Au nanocluster supported on CeO₂(111) surface and steps,
 - Au-CeO₂ interface supplies oxygen for CO oxidation
- 2) Selective CO oxidation by CuO_x supported TiO₂ cluster,
 - Ti-Cu(111) and Ti-Cu₂O(111) interfaces selectively oxidize CO
- 3) Pt/CeO₂/TiO₂ composite catalyst.
 - CeO₂-TiO₂ interface stabilizes extremely small Pt clusters (or atoms)

These results demonstrate how the interfaces can be utilized for better catalysts with excellent Reactivity, Selectivity, and Stability.