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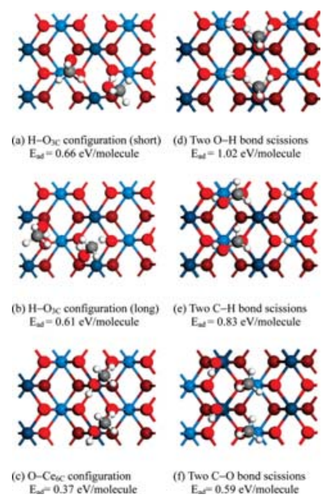
Science Made Possible

Atom-level study shows how methanol interacts with catalyst

Supercomputers used to study inexpensive metal oxide catalyst for hydrogen fuel production

With sophisticated computer simulations, scientists from Pacific Northwest National Laboratory's Institute for Interfacial Catalysis and Southern Illinois University showed how an inexpensive metal oxide catalyst can decompose methanol (CH_3OH) to produce hydrogen. Methanol adsorption and decomposition over a ceria catalyst, without depositing precious transition metals, could serve as a promising alternative catalyst. To make the hydrogen economy a reality, the atomic-level chemical and physical phenomena in the catalysts that drive the desired reactions must be understood. This theoretical research provides insight into methanol dissociation on ceria catalyst surfaces and provides information for developing effective low-cost catalysts.



Modeling bond scissions

The team showed that for 0.25 monolayer coverage, breaking of the C–H bond produces the most stable products, but breaking the O–H bond is kinetically favored. The O–H bond breaking was almost spontaneous on CeO_2(111) and CeO_2 (110) surfaces. When coverage was increased to 0.5 monolayers, the O–H bond scission became thermodynamically and kinetically favorable. At full monolayer coverage, only molecular adsorption of methanol was predicted. The results are consistent with earlier experiments, but explain the molecular details of adsorption and dissociation that could not be observed experimentally.

This work was done with the supercomputer and VASP software in the Department of Energy's Environmental Molecular Sciences Laboratory and the National Energy Research Scientific Computing Center.

Scientific impact: This study provides new insights into the nature of alcohol decomposition chemistry over metal oxide surfaces, part of EMSL's ongoing work to design and control material synthesis.

Societal impact: As the financial and environmental costs of oil use continue to rise, cleaner-burning domestic fuels, such as hydrogen, are needed. To make manufacturing hydrogen a reality requires effective affordable catalysts, and this work supports understanding and eventually designing these catalysts.

For more information, contact EMSL Communications Manager Mary Ann Showalter (509-371-6017).

Citation: Mei DH, NA Deskins, M Dupuis, and QF Ge. 2008. "Density Functional Theory Study of Methanol Decomposition on the CeO_2(110) Surface." *Journal of Physical Chemistry C* **112**(11):4257-4266.

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