Large or small, platinum clusters provide new insights

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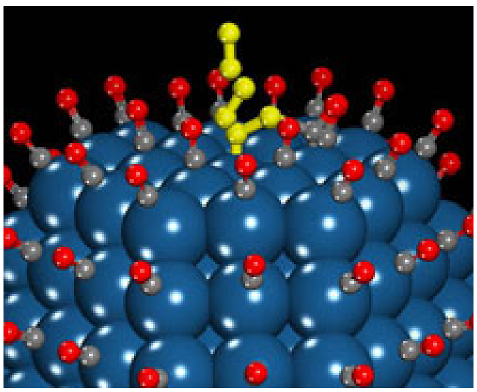

Density functional theory calculated reaction path for formation of the reactive O*-O-C*=O intermediate, the kinetically relevant step for CO oxidation at low temperature.

Using Environmental Molecular Sciences Laboratory's high-performance supercomputing capabilities, scientists helped resolve longstanding controversies about the effect of platinum cluster size on some emissions-reducing reactions in automobile catalysts.

The research team included scientists from the University of California, Nanostellar, Inc., the University of Virginia and Lawrence Berkeley National Laboratory.

Carbon monoxide (CO) removal from combustion exhaust, typically carried out by oxidation on three-way catalysts containing platinum, is critically important for cleaner-burning engines.

The researchers used EMSL's Chinook supercomputer to carry out detailed *ab initio* quantum mechanical calculations on very large (201-atom) platinum clusters to model the environment of platinum nanoparticles fully covered with CO.

The team integrated rigorous kinetic, isotopic, and in-situ spectroscopy studies of platinum clusters with theoretical simulations of CO oxidation catalysis at conditions prevalent in many industrial applications to gain a better understanding of catalytic activity on platinum clusters.

When a platinum catalyst covered with CO is at low temperatures, the size of the platinum cluster makes little difference in the rate of oxidation.

For other reactions catalyzed by platinum clusters in automobile exhaust, larger clusters will oxidize nitric oxide or dimethyl ether much faster.

CO oxidation is also a critical step in the production of pure hydrogen streams for use in fuels cells and in many chemical processes.

More information: Allian AD, et al. 2011. "Chemisorption of CO and Mechanism of CO Oxidation on Supported Platinum Nanoclusters." *J. Am. Chem. Soc.*, 2011, 133 (12), pp 4498–4517 DOI: 10.1021/ja110073u

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