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Catalytic reactions on Pt nanoclusters: Size and coverage effects in CO oxidation and methanol decomposition

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Platinum nanoclusters are widely used as catalysts for various processes, such as oxidation reactions and catalytic reactions of organic molecules. To optimize the performance of the platinum catalyst it is important to understand the mechanisms of the catalytic reactions on a molecular level and to investigate how various parameters of the clusters, such as cluster's size and shape, affect the rate of the reaction and the efficiency of the catalyst. In the current work, CO oxidation and methanol decomposition on platinum nanoclusters of various sizes and shapes were studied using the density functional theory (DFT). Obtained results are used to understand the role of various adsorption sites on the cluster and the differences between the various facets. The results of calculations suggest that clusters between one and two nm in size may provide better conditions for CO oxidation than clusters of other sizes, in agreement with previously published experimental data. However, methanol decomposition may occur faster on larger clusters.

Biography

Sergey Dobrin obtained his Master's Degree in Physics from the Moscow Institute of Physics and Technology in the area of Laser Physics. He completed Ph.D. studies at the Institute of Physical Chemistry, Polish Academy of Sciences in Warsaw. His research was devoted to photophysics and spectroscopy of organic molecules. Later he studied photoinduced reactions on solid surfaces in the group of Professor Polanyi at the University of Toronto, and conducted theoretical research of the catalytic reactions on solid surfaces and nanoparticles at the Center for Atomic-scale Materials Design (Director Professor Nørskov) at the Danish Institute of Technology. Currently he works on theoretical modeling of the formation of metal nanoclusters on silicon surfaces and chemical reactions on metal nanoclusters at the University of Toronto.

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