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Computational studies of H2, O2, and CO adsorption on Pt and Pt-Ru catalyst clusters for hydrogen fuel cell applications

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Computational Studies of Platinum and Platinum-Ruthenium Alloy Catalysts for Hydrogen Fuel Cells

Previous computational studies of hydrogen fuel cell catalysis primarily focus on single adsorbate and therefore do not reflect the realistic situation. Here we investigated the effect of multiple hydrogen, oxygen, and carbon monoxide adsorption on bimetallic nanoclusters as allowed by computational resources. The criteria of which we studied were adsorption energies, electron densities, electrostatic charges, and HOMO-LUMO energy gaps with respect to each structure. We found that Pt-Ru clusters have better performance than pure Pt clusters early in the adsorption course, and pure Pt clusters are more consistent than Pt-Ru clusters in a sequence of adsorbate introduction.

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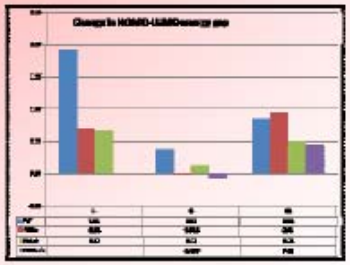
Introduction

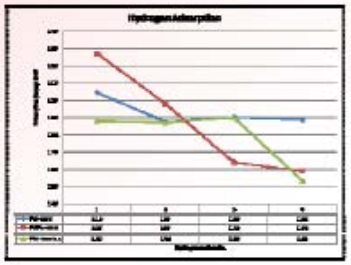
We present density functional theory (DFT) calculations of chemisorption of H_2, O_2, and CO molecules on pure platinum (Pt_4) and platinum-ruthenium clusters (Pt_3Ru) of tetrahedral and rhombus configurations. Unlike most previous computational studies of hydrogen fuel cell catalysis in which the interaction of a single adsorbate molecule with the catalyst cluster was investigated, we explore the effect of co-adsorbed molecules on the catalytic activity. Adsorption energy, HOMO-LUMO energy gap, and electrostatic potential map of each metal-adsorbate system were calculated to investigate the effect of adsorbate saturation on the catalyst particle.

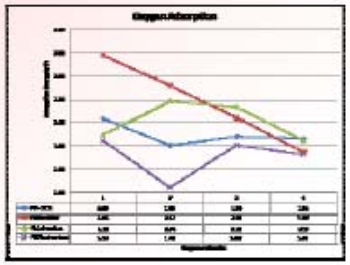
Method

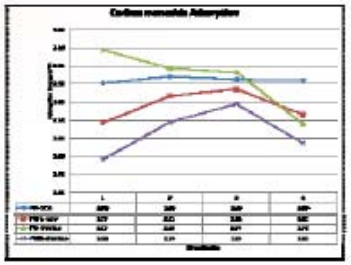
DFT calculations were performed using the DMol^3 software with the Perdew-Wang exchange-correlation functional. Double numerical basis set with polarization functions were adopted to evaluate the total energy and relevant properties of each geometrically optimized structure.

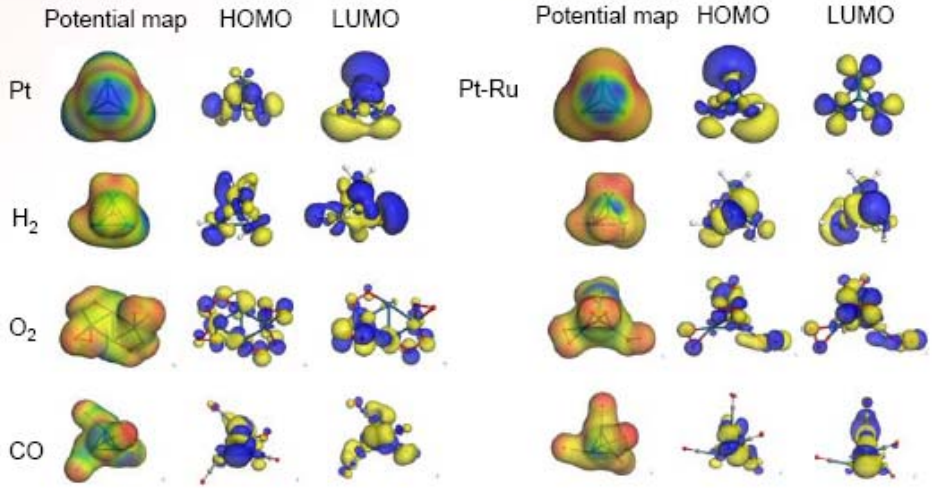
Results

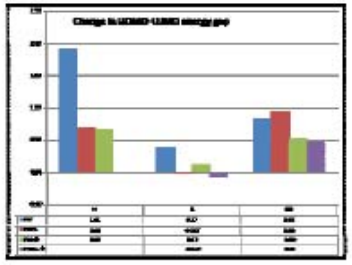












Conclusion

Results show that the doping of Ru into tetrahedral Pt structure raises the adsorption energy initially for hydrogen and oxygen interactions. However, Ru doping causes a decrease in the adsorption energy after four adsorbates while that of pure Pt remains nearly constant during the adsorption process. For CO adsorption, the doping of Ru lowers the adsorption energy for all four CO molecules interacting with the cluster. This shows that Ru-doped clusters may be less susceptible to CO poisoning because the adsorbed CO molecules can be easily desorbed at lower temperatures.

Acknowledgment

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