

Size Effect of AgCu Bimetallic Nanoparticles on Catalytic Activity in the PEMFC Cathode

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As an oxygen reduction reaction (ORR) catalyst in the proton exchange membrane fuel cell (PEMFC) cathode, Pt is still the best even though numerous experimental and theoretical researches are being performed to find its substitute or reduce its amount.

Previously, we performed the density functional theory (DFT) calculations to describe the ORR activity of AgCu bimetallic nanoparticles (NPs) in different sizes (13 and 38 atoms) using adsorption energy and oxygen dissociation energy barrier in our previous researches^{2,3}. In this study, we calculate catalytic properties of larger AgCu bimetallic NPs composed of 55 atoms and try to find the size effect, if any.

In conclusion, we found out that adsorption energy of oxygen and dissociation energy barrier are strongly correlated with the size of NP itself. The proper size of NP is found essential to maximize the catalytic activity.

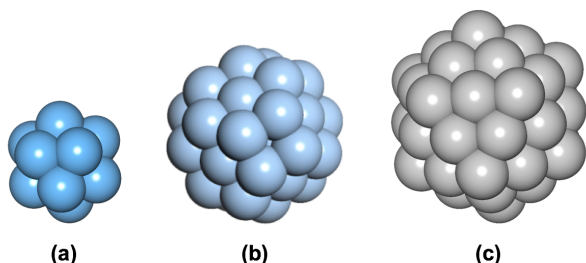


Fig.1 Various size of NP systems we prepared for this work. (a) 13, (b) 38, (c) 55 atoms/NP

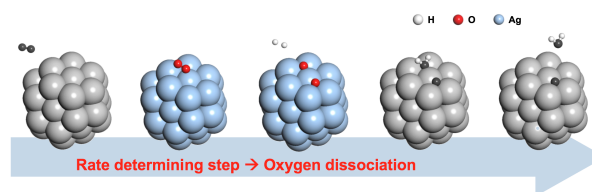


Fig.2 Schematic diagram of dissociative pathway of ORR and its rate determining step

References

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