

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Two dimensional N-containing carbon materials for oxygen reduction reaction YEXIN FENG, ZHENPENG HU, LIXIN ZHANG, School of Physics, Nankai University — Seeking Pt replacement catalysts for cathode oxygen reduction reaction (ORR) is very important for the application of some new energy technologies like fuel cells and lithium-air batteries. N-doped graphene and carbon nitride sheets are two kinds of promising materials. For the N-doped graphene, it is found that nitrogen clusters other than isolated substitutionals are the active sites for oxygen reduction. Clusters with three or four N atoms are found to be the most active. Codoping boron (or Fe, Co) can effectively stabilize these high energy clusters while keep the cluster's high activity. For the carbon nitride sheets, in the C:N ratio range of 2.0-3.0, they are stable enough and can potentially catalyze the oxygen reduction as efficiently as Pt. It is revealed that the concentration of nitrogen can tune the Fermi level of the material and thus the catalytic property. The catalytic sites are located at those carbon atoms with special configurations rather than the nitrogen atoms. These results are helpful in designing N-containing carbon materials for ORR.

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Date submitted: 31 Oct 2012

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