The Study on Vacancy Effect of the Heteroatom Doping of Graphene : Insight from DFT

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The electrocatalysts used for ORR in PEMFC should satisfy thermodynamic stability and catalytic activity. Moreover, it is also important to the uniform dispersion in the MEA preparation. The main limitation is that the ionomer agglomeration around Pt as Pt/C slurry is sprayed or coated on film. As a result, it is a barrier to the mass transfer of oxygen, which reduces the overall MEA performance. We have tried to improve the stability and activity of the electrocatalysts by doping S or P into graphene structures with vacancies. By using DFT, we calculated the formation energy of each structure generated from 0 to 100 at% of the dopant and vacancies by using the cluster expansion method. And we found a stable structure by drawing a convex hull. The adsorption energy was calculated by binding ionomers or Pt on the heteroatom doping graphene with the vacancies, which was previously defined. Also, the activity and stability of Pt on heteroatom doping graphene could be identified by exploring electronic structures. As a result, it provided insights into the activity and stability of the support by adding vacancies to heteroatom doping graphene.