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Author: Ms. Simranjit Grewal
The National AeroSpace Training And Research Center (THE NASTAR CENTER), United States, sgrewal7@ucmerced.edu

Ms. Angela Macedo Andrade
University of California, Merced, United States, amacedoandrade@ucmerced.edu
Mr. Alireza Karimaghaloo
University of California, Merced, United States, akarimaghaloo@ucmerced.edu

GRAPHENE FUNCTIONALIZATION USING TRANSITION METAL OXIDE FOR ENHANCING THE BIFUNCTIONAL CATALYTIC ABILITY OF NANOPARTICLES

Abstract

Regenerative Fuel Cells (RFS) used for NASA's aerospace vehicles require tri-functionality as more materials used for space exploration increases weight, thereby, increasing cost. Tri-functionality would require the ability to supply energy using oxygen reduction reactions (ORR), oxygen evolution reactions (OER) and hydrogen evolution reactions (HER), allowing both water formation and splitting. Noble metals such as Pt and its alloys (Pt/Ir or Pt/Ru) have been routinely used as RFS due to an efficient catalytic active surface area, selectivity towards oxygen and hydrogen, and stability in harsh environments, but their susceptibility to agglomeration, fast degradation and methanol poisoning have driven researchers to find alternatives [1]. Non-precious transition metal oxides (TMO) including Fe3O4, MnOx and Co3O4 have attracted significant attention as they maximize catalytically active sites per volume and mass [2].

We employ a hybrid structure where ZrO2 or TiO2 is deposited/decorated on a highly 3D conductive carbon structure that leverages extremely high surface area and excellent electronic conductivity like graphene oxide (GO). However, GO only has O-containing functional groups on the wrinkles and edges for nanoparticle binding while its basal plane stays relatively non-reactive. Therefore, we functionalize the basal surface of GO using hydrobromic and/or oxalic acid to create hydroxyl and/or carboxyl groups, respectively. Once treated, the GO was hydrothermally reacted with precursors (ZrOCl2) or nanoparticles (P25).

The hydroxylated ZrO2/GO hybrids showed the best ORR and OER performance in 0.1 M KOH, in terms of current density, electron transfer number and onset/half-wave potential as it was comparable to the performance of Pt/C. From a series of experimental analyses, a strong tethering of metal oxide particles on the basal plane of graphene prohibits restacking, and that the particle-graphene interfaces (as opposed to the particle or graphene itself) dictates the performance and reaction route, as seen in density function theory calculations. However, further analysis was needed if an additive such as PdO2 via hydrothermal reaction could be used to increase HER capabilities [3]. Results have indicated an increase in HER capabilities of the ZrO2/GO/PdO2 hybrid.

References

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