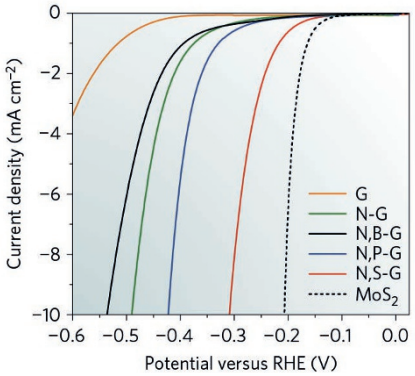
Nature Reviews Chemistry | Published online 29 Mar 2018; doi:10.1038/s41570-018-0138

IN BRIEF

HETEROGENEOUS CATALYSIS

How heteroatom-doped graphenes make hydrogen faster



Adapted from Jiao, Y. et al. (2016), Macmillan Publishers Limited.

Metal-free carbon materials, such as those derived from graphene, make attractive alternatives to metal-containing electrocatalysts owing to the high natural abundance of the constituent elements and their potentially lower cost. However, the catalytic activities of metal-free materials are typically inferior to those of traditional metal-based electrocatalysts. Shi-Zhang Qiao and colleagues address this issue by linking the electrocatalytic hydrogen evolution activity of a series of doped graphene materials to reaction energetics computed with density functional theory. Their recent work in *Nature Energy* explores the effect of doping graphene with either one or two elements. A key finding is that in both singly-doped and doubly-doped materials, the most active catalytic sites are the carbon atoms adjacent to the dopant atoms. Based on their investigation of the catalytic activities, it is predicted that tuning the doping level and the surface area of the 2D catalyst will afford a metal-free catalyst with activity rivalling the benchmarks set by metal-containing species.

James Gallagher, Associate Editor, Nature Energy

ORIGINAL ARTICLE Jiao, Y. et al. Activity origin and catalyst design principles for electrocatalytic hydrogen evolution on heteroatom-doped graphene. *Nat. Energy* **1**, 16130 (2016)