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DFT Studies of the ORR Activity of Carbon Encapsulated Fe_3C

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CarbonbasedcatalystscontainingFe-N_4C_N active sites have shownactivity for the oxygenreductionreaction (ORR) comparable to platinum in acidelectrolytesatlowcurrentdensities.[1–3]Thesecatalysts, however,requirehighloading to achievethe currentdensitiesdesiredfor fuel cell applications. Improvements in volumetricactivity are thereforeneeded to the reducemass transport limitations of the thickcatalyst layer.Furthermore, long-termstability and suppression of H_2O_2selectivityneed to beaddressed.Graphite encapsulated Fe_3C wasrecentlysuggested to be a durable ORR catalystwithoutnitrogencontaining active sites.[2]
Here,we use atomic-scaledensityfunctionaltheory to investigatethe pathway for O_2reduction to H_2O_2 and H_2O on extended model surfaces of a Fe_3C-graphite catalyst in order to elucidateeffects of catalyst doping, strain, thickness and quality of the encapsulatinggraphiticlayers.
Wefind Fe_3C significantlyincrease the activity of graphite zigzag edges, whereasthe activity of nitrogen free graphite basal planes iscomparativelyunaffected by the presence of Fe_3C.

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