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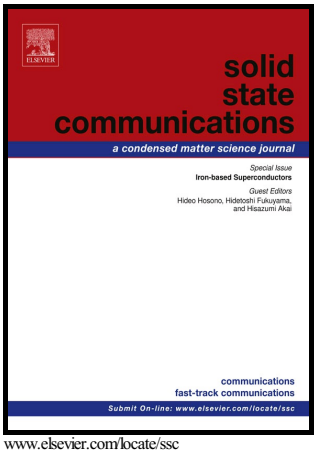
Yang Li, Chunyang He, Lixin Zhang



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PII: S0038-1098(17)30288-0
DOI: http://dx.doi.org/10.1016/j.ssc.2017.09.005
Reference: SSC13272

To appear in: *Solid State Communications*

Received date: 12 June 2017
Revised date: 31 August 2017
Accepted date: 1 September 2017

Cite this article as: Yang Li, Chunyang He and Lixin Zhang, Identify and form the active sites in sulfur-doped graphene for oxygen reduction reaction: The key of the dissociated O_2 adsorption, *Solid State Communications,* http://dx.doi.org/10.1016/j.ssc.2017.09.005

Identify and form the active sites in sulfur-doped graphene for oxygen reduction reaction: The key of the dissociated O_2 adsorption

Yang Li, Chunyang He and Lixin Zhang*

School of Physics, Nankai University, Tianjin 300071, People's Republic of China

lxzhang@nankai.edu.cn

Abstract

Sulfur (S) doping in graphene is studied using first-principles calculations. The S dopants can assume various configurations such as graphitic-S, pyridinic-S, and pyrrolic-S, and prefer to locate at the graphene edges. Oxygen molecules (O_2) can be adsorbed on the S dopants at the edges, but with much larger adsorption energies than required for catalyzing the oxygen reduction reaction. We found an energetically favored three-pyridinic-S cluster in bulk graphene, on which the O_2 adsorption energies are much reduced and comparable to that on the Pt (111) surface. This is due to a confinement effect, which could be considered a key rule in doping graphene for potential applications.

Graphical abstract

The sulfur clusters can be synthesized during the growth of graphene and are the possible active sites for oxygen reduction reaction.