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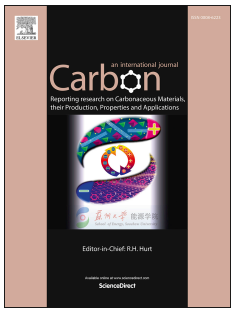

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Topological Line Defects in Graphene for Applications as Gas Sensing

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Abstract

Topological line defects in graphene synthesized in a highly controlled manner open up new research directions for nanodevice applications. Here, we investigate two types of extended line defects in graphene, namely octagonal/pentagonal and heptagonal/pentagonal reconstructions. A combination of density functional theory and non-equilibrium Green's function methods was utilized in order to explore the application potential of this system as an electronic gas sensor. Our findings show that the electric current is confined to the line defect through gate voltage control, which combined with the enhanced chemical reactivity at the grain boundary, makes this system a highly promising candidate for gas sensor applications. As a proof of principle, we evaluated the sensitivity of a prototypical device toward NO_2 molecule, demonstrating that it is indeed possible to reliably detect the target molecule.

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