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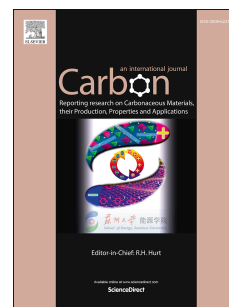
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Tribochemistry of graphene on iron and its possible role in lubrication of steel

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Abstract

Recent tribological experiments revealed that graphene is able to lubricate macroscale steel-on-steel sliding contacts very effectively both in dry and humid conditions. This effect has been attributed to a *mechanical action* of graphene related to its load-carrying capacity. Here we provide further insight into the functionality of graphene as lubricant by analysing its *tribochemical action*. By means of first principles calculations we show that graphene binds strongly to native iron surfaces highly reducing their surface energy. Thanks to a passivating effect, the metal surfaces coated by graphene become almost inert and present very low adhesion and shear strength when mated in a sliding contact. We generalize the result by establishing a connection between the tribological and the electronic properties of interfaces, which is relevant to understand the fundamental nature of frictional forces.

1. Introduction

In recent years the search for novel lubricant materials and coatings has gained increasing importance to face the massive economic and environmental costs related to friction and wear. Furthermore, the development of miniaturized devices with high surface-to-volume ratio, such as micro- and nano-electromechanical systems, quests for new solutions for tribological problems like stiction that seriously undermine their functionality. Graphene is

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