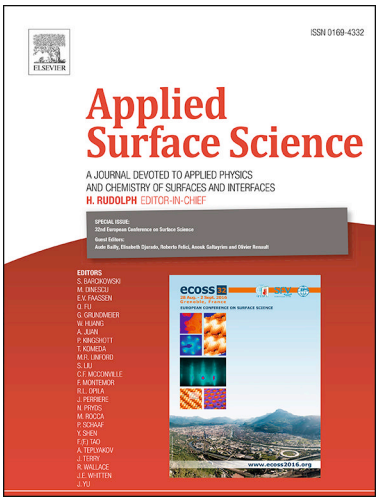

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Effect of uniaxial stress on the electrochemical properties of graphene with point defects

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Abstract

We report a calculational study of electron states and the resulting electrochemical properties of uniaxially strained graphene with point defects. For this study the reduction of ferricyanide to ferrocyanide serves as a benchmark electrochemical reaction. We find that the heterogeneous electron transfer activity of the perfect graphene electrode rises under uniaxial strain. However, evolution of the cathodic reaction rate depends on the direction of strain. For moderate lattice deformations, the zigzag strain improves electrochemical performance better than the armchair strain. Standard rate constant increases by 50% at the zigzag strain of 10%. Vacancies, covalently bonded moieties, charged adatoms and substitutional impurities in the zigzag strained graphene induce changes in the shape of the curve of the cathodic reaction rate. However, this changes do not translate into the the electrocatalytic activity. Vacancies and covalently bonded moieties at concentration of 0.1% do not affect the electrochemical performance. Charged adatoms and substitutional impurities give a slight increase in the standard rate constant by, respectively, 2.2% and 3.4%.

Keywords: graphene, uniaxial strain, point defects, density of states, heterogeneous electron

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