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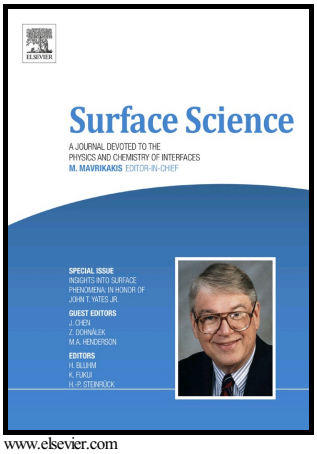

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Phenol Dissociation on Pristine and Defective Graphene

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Abstract

Phenol (C_6H_5O–H) dissociation on both pristine and defective graphene sheets in terms of associated enthalpic requirements of the reaction channels was investigated. Here, we considered three common types of defective graphene, namely, Stone-Wales, monovacancy and divacancy configurations. Theoretical results demonstrate that, graphene with monovacancy creates C atoms with dangling bond (unpaired valence electron), which remains particularly useful for spontaneous dissociation of phenol into phenoxy (C_6H_5O) and hydrogen (H) atom. The reactions studied herein appear barrierless with reaction exothermicity as high as 2.2 eV. Our study offers fundamental insights into another potential application of defective graphene sheets.

Keywords: density functional theory (DFT), nudged elastic band (NEB), graphene, phenol, phenoxy, Stone-Wales, vacancy defects

1. Introduction

Phenol (C_6H_5OH), a planar aromatic compound with singular hydroxyl group (OH), has ubiquitous industrial and pharmaceutical applications. It widely serves in the production of