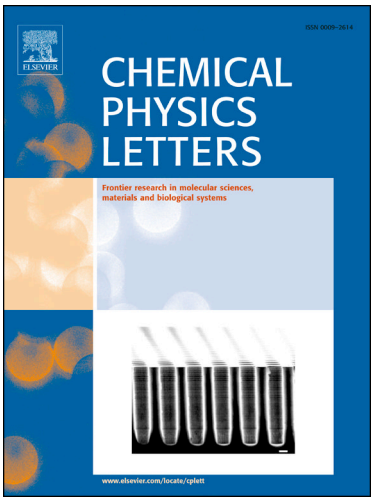

Frontiers article

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Coupled Cluster and Density Functional Investigation of the Neutral Sodium-Benzene and Potassium-Benzene Complexes

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Abstract

By means of coupled-cluster calculations we studied the neutral complexes: Na-benzene and K-benzene. They are non-ionic presenting C_{6v} symmetry. In contrast with the results obtained for Li-benzene, the non-ionic C_{2v} structure was not a minimum. At the CCSD(T)/CBS level of theory, with the inclusion of relativistic and core-valence effects, the dissociation energies for sodium and potassium benzene complexes are 2.4 and 3.3 kcal/mol, respectively. We found that most density functionals overestimate the adsorption energies of alkalis onto benzene. Therefore, special caution must be taken when DFT methods are employed to investigate the interactions between these elements and carbon nanomaterials.

Keywords: carbon nanomaterials, adsorption, graphene, density functional calculations, batteries.

1. Introduction

We are mostly relying on fossil fuels to meet our energy requirements [1]. This is the main cause of CO_2 increase in our environment. For example, the European Union imports 750 million of euros per day of fossil fuels [1]. For this reason, it has been estimated by the United Nations that if the emissions of greenhouse gasses such as CO_2, etc; do not decline, the temperature of the planet could rise by more than 4 °C by the end of this century [2]. As a consequence, it is essential to reduce our dependency on the fossil fuels. The contributions of hydroelectric, nuclear, thermal and eolic energies to the global energy consumed in the planet have been increased [1]. For example, in 2017 renewable sources contributed to 30% of the energy consumed in Europe [1]. However, since efficient energy storage