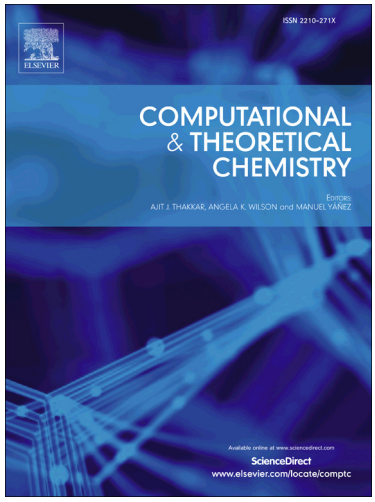

Adsorption on a nanoporous organic polymer for clean energy applications: A multiscale modeling study using Density Functional Tight Binding Approach

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PII: S2210-271X(16)30541-2
DOI: http://dx.doi.org/10.1016/j.comptc.2016.12.037
Reference: COMPTC 2354

To appear in: *Computational & Theoretical Chemistry*

Received Date: 4 November 2016
Revised Date: 22 December 2016
Accepted Date: 25 December 2016

Please cite this article as: A. Domínguez-Castro, F. Guzmán, Y. Novo-Fernández, Adsorption on a nanoporous organic polymer for clean energy applications: A multiscale modeling study using Density Functional Tight Binding Approach, *Computational & Theoretical Chemistry* (2016), doi: http://dx.doi.org/10.1016/j.comptc.2016.12.037

Adsorption on a nanoporous organic polymer for clean energy applications: A multiscale modeling study using Density Functional Tight Binding Approach.

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KEYWORDS: adsorption, ferrocenyl-nanoporous network, SCC-DFTB, MD simulation.

ABSTRACT:

Adsorption of carbon dioxide, methane and hydrogen on the novel ferrocenyl-nanoporous organic polymer was studied from an approximate density-functional method. Geometric, energetic and electronic parameters are obtained using the self-consistent charge density functional tight binding (SCC-DFTB) spin polarized approach and prove a mechanism of adsorption governed by physisorption processes. In order to gain a deeper understanding of the effect of temperature on the adsorption-desorption process, an SCC-DFTB / MD simulation is implemented which enabled a satisfactory agreement with the experimental results reported in the literature.