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Adrian Domínguez-Castro, Fernando Guzmán, Yasser Novo-Fernández

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

Adrian Domínguez-Castro[‡], Fernando Guzmán^{‡,}, Yasser Novo-Fernández[‡]*

[‡] Higher Institute of Technologies and Applied Sciences (InSTEC), Quinta de los Molinos, Ave. Salvador Allende, corner Luaces, Plaza de la Revolución, Havana, Cuba.

* Corresponding author

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.

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