

Adsorption of PET on Concrete Nano-Structures: An In-Silico Assay

L. Bárcenas¹, F. Aguilera-Granja², G. Ramírez-García³, E. Díaz-Cervantes^{1*}

¹Departamento de Alimentos, Centro Interdisciplinario del Noreste (CINUG), Universidad de Guanajuato, 37975 Tierra Blanca, Guanajuato, México. tl.barcenasramirez@ugto.mx* e.diaz@ugto.mx*

²Instituto de Física, Universidad Autónoma de San Luis Potosí, 78000 San Luis Potosí, SLP, México

³Cátedras CONACYT-Centro de Investigación en Química Aplicada, COITTEC, 140, Blvd. Enrique Reyna, Saltillo, Coahuila 25294, México.

Abstract - The present work analyses the first approach of the use of PET as a component of a sustainable alternative to generate an enforced concrete. Through the computational study of one nanostructured concrete model and two monomers PET system, the adsorption energies of PET on concrete were evaluated in the present work, which was exergonic (-7.67 eV) and therefore can be formulated as a perspective a sustainable concrete using one of the principal waste in the world, applied to the construction industry.

Keywords: PET, Concrete, Nano-structures, Adsorption-energy, DFT