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E. Nosedá Grau, G. Román, A. Díaz Compañy, G. Brizuela, A. Juan, S. Simonetti

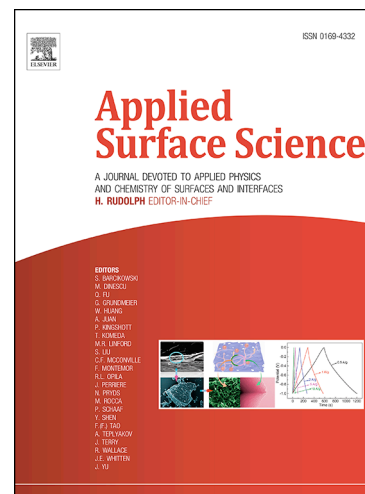
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**SURFACE MODIFICATION VS SORPTION STRENGTH: STUDY OF
NEDAPLATIN DRUG SUPPORTED ON SILICA**

E. Nosedá Grau^{1,2}, G. Román¹, A. Díaz Compañy^{1,2}, G. Brizuela¹, A. Juan¹, S. Simonetti^{1,3}

¹Instituto de Física del Sur (IFISUR), Departamento de Física, Universidad Nacional del Sur (UNS),
CONICET, Av. L. N. Alem 1253, B8000CPB - Bahía Blanca, Argentina.

²Comisión de Investigaciones Científicas (CIC), Calle 526 e/10 y 11, 1900 – La Plata, Argentina.

³Universidad Tecnológica Nacional (UTN), 11 de Abril 461, B8000LMI - Bahía Blanca, Argentina.

E-mail: ssimonet@uns.edu.ar

Abstract

The interaction of nedaplatin drug with modified SiO₂(001) surfaces has been investigated within the framework of Density Functional Theory. Nedaplatin molecule is adsorbed spontaneously onto silica surfaces. Silica surface prevents drug degradation allowing the chemical attachment without any impact on the drug structure itself. The nedaplatin sorption is mainly governed by H-bonding interactions on hydrated and trimethylsilane-functionalized surfaces, while the drug is major stabilized by N-O, O-O interactions and H partial dissociation on dehydrated silica. The differences on the adsorption strength could be used in future studies to control the drug release, developing delivery silica systems according therapy requirements.

Keywords: drug delivery; nedaplatin; silica; adsorption; DFT

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