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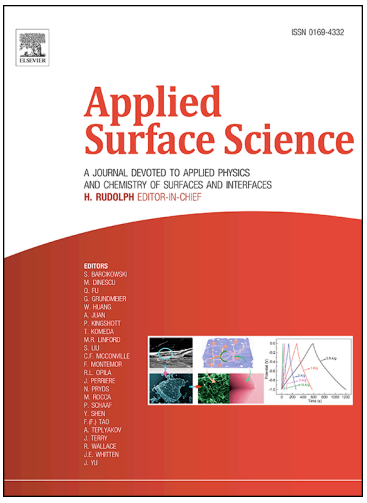

Full Length Article

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

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PII: S0169-4332(18)32646-1
DOI: https://doi.org/10.1016/j.apsusc.2018.09.213
Reference: APSUSC 40517

To appear in: *Applied Surface Science*

Received Date: 26 August 2018
Revised Date: 23 September 2018
Accepted Date: 25 September 2018

Please cite this article as: E. Noseda Grau, G. Román, A. Díaz Compañy, G. Brizuela, A. Juan, S. Simonetti, SURFACE MODIFICATION VS SORPTION STRENGTH: STUDY OF NEDAPLATIN DRUG SUPPORTED ON SILICA, *Applied Surface Science* (2018), doi: https://doi.org/10.1016/j.apsusc.2018.09.213

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

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Abstract

The interaction of nedaplatin drug with modified SiO_2(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-fuctionalized 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