

p-nitrobenzoic acid adsorption on nanostructured gold surfaces investigated by combined experimental and computational approaches.

Autorzy

Jarosław J. Panek
Aneta Jezierska-Mazzarello
Aleksander Koll
Galina Dovbeshko
Olena Fesenko

Rok wydania

2011

Czasopismo

ChemPhysChem

Numer woluminu

12

Strony

2485-2495

DOI

10.1002/cphc.201100067

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Adsorption of guest molecules on host surfaces can lead to dramatic changes in the spectral properties of the guest. One such effect is surface-enhanced infrared absorption (SEIRA), observed when the guest is adsorbed on, for example, thin films, metal surfaces, or nanotubes. p-Nitrobenzoic acid (p-NBA) exhibits a SEIRA effect when adsorbed on Ag and Au. Herein, the IR spectra of p-NBA adsorbed on a homemade rough Au surface, recorded in reflection mode with an angle of incidence of 16.5°, are reported. This SEIRA experiment reveals more bands than found by previous SEIRA studies. The intensities of both symmetric and asymmetric COO(-) and NO(2) stretching, in-plane CH, and C=C ring stretching modes are enhanced. Theoretical models constructed on the basis of density functional theory reveal the binding mode of p-NBA to gold "particles". The p-NBA anion binds to gold much more strongly than the neutral form, and interaction via the carboxylic oxygen atoms is preferred over the nitro group-gold contact. A significant charge transfer during chemisorption is found, which is considered to be crucial in leading to a high SEIRA enhancement factor.

Adres publiczny

<http://dx.doi.org/10.1002/cphc.201100067>

Strona internetowa wydawcy

onlinelibrary.wiley.com