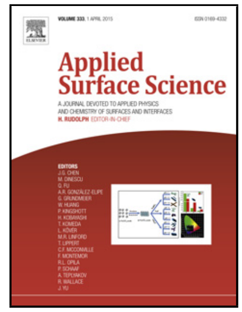
Accepted Manuscript

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| PII: | S0169-4332(15)00746-1 |
| DOI: | http://dx.doi.org/doi:10.1016/j.apsusc.2015.03.150 |
| Reference: | APSUSC 30027 |
| To appear in: | *APSUSC* |
| Received date: | 7-2-2015 |
| Revised date: | 23-3-2015 |
| Accepted date: | 23-3-2015 |

Please cite this article as: C. Qiu, Y. Xing, W. Yang, Z. Zhou, Y. Wang, H. Liu, W. Xu, Surface Molecular Imprinting on Hybrid $SiO_2$-Coated CdTe Nanocrystals for Selective Optosensing of Bisphenol A and Its Optimal Design, *Applied Surface Science* (2015), http://dx.doi.org/10.1016/j.apsusc.2015.03.150

# Surface Molecular Imprinting on Hybrid $SiO_2$-Coated CdTe Nanocrystals for Selective Optosensing of Bisphenol A and Its Optimal Design

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Highlights

Molecular dynamics simulation was employed to optimize the imprinting shell of the fluorescent sensor.

Hybrid $SiO_2$-coated CdTe were synthesized to enhance the sensitivity and selectivity of the sensor.

Imprinting factor of 4.56 and detection limit of 6nmol $L^{-1}$ for BPA were obtained.

The sensor was applied to determine the concentration of BPA in river water and milk.

Abstract

Twenty molecular dynamics (MD) simulations of molecular imprinting prepolymerization systems had been performed to optimize the imprinting shell of the fluorescent sensor. The results revealed that the system with a Bisphenol A (BPA): 3-aminopropyltriethoxysilane (APTES): tetraethylorthosilicate (TEOS) mole ratio of 10:15:60 had the most stable template (T)-functional monomer (FM) cluster. Correspondingly, five kinds of imprinted and non-imprinted polymers were synthesized to assess the reliability and validity of the simulation results. Hybrid $SiO_2$-coated CdTe NCs (HS-QD) were synthesized by a simple reflux procedure including a sol-gel reaction that resulted in the formation of a hybrid $SiO_2$ layer with CdS-like clusters on a CdTe core. Based on the optimal component ratio of the prepolymerization system, MIP shells were anchored on the surface of HS-QD to build a fluorescent MIP sensor. A linear relationship between relative fluorescence intensity and the concentration of BPA had been obtained covering the concentration range of 0.05-10 μmol $L^{-1}$ with a limit of detection of 6 nmol $L^{-1}$. The feasibility of the fluorescent sensor was successfully evaluated through the analysis of BPA in river water and milk. The recoveries is above 96.31%, and the relative standard deviation (RSD) ranged from 1.55%-2.78%.