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ABSTRACT BOOK

A Mesoporous Zirconia Coating for Sensing Applications using ATR-FTIR Spectroscopy

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Mid-infrared attenuated total reflection (ATR) spectroscopy is a powerful tool for in situ monitoring of various processes. Mesoporous silica is an extensively studied material and has already been applied in sensing schemes due to its high surface area and tunable surface chemistry1. However, the poor chemical stability in aqueous solutions at pH values higher than 8 as well as the strong absorption below 1250 cm^{-1} limits the range of applications. Therefore, a mesoporous zirconia coating on ATR crystals was developed to circumvent these problems. The synthesis, surface modification and characterization of ordered mesoporous zirconia films on Si-wafers and Si-ATR crystals are presented. Cubic films with a thickness of 237 nm were obtained. The surface of the zirconia coating was modified using trichloro(phenyl)silane and applied in sensing schemes using aromatic and aliphatic nitriles in aqueous solution as organic pollutants. X-ray diffraction (XRD) studies confirm a high thermal stability of the mesoporous structure up to 900°C and for 24 h at 500°C. The mesoporous zirconia coating shows a high chemical resistance when keeping it in alkaline solution with a pH-value of 12 for 72 h. The success of surface modification is confirmed by FTIR spectroscopy and contact angle measurements. Traces of benzonitrile and valeronitrile in water are used as model analytes to evaluate the enrichment performance of the film. The experimental results are fitted using Freundlich isotherms and enrichment factors of 162 and 26 are calculated for 10 mg L^{-1} benzonitrile and 25 mg L^{-1} valeronitrile in water, respectively. Limits of detection of 1 mg L^{-1} for benzonitrile and 11 mg L^{-1} for valeronitrile are obtained. After the enrichment the sensing layer was completely regenerated by flushing with water. The high thermal and chemical stability of this coating allows the application in fields other than sensing like catalysis with the possibility of in situ monitoring using FTIR spectroscopy.

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[1] Baumgartner, B.; Hayden, J.; Schwaighofer, A.; Lendl, B., In Situ IR Spectroscopy of Mesoporous Silica Films for Monitoring Adsorption Processes and Trace Analysis. Acs Appl Nano Mater 2018, 1 (12), 7083-7091.

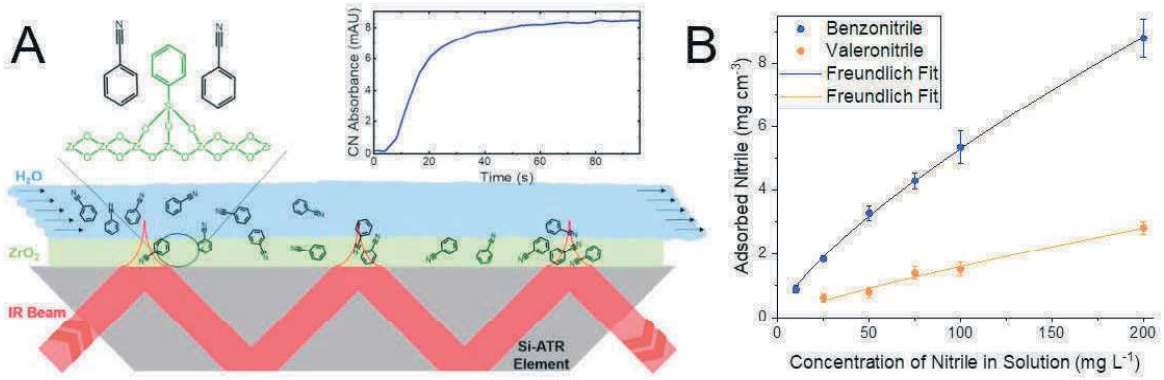

Figure 1. (A) Enrichment of an aqueous benzonitrile solution using a phenylsilylated ZrO2-coating on a Si-ATR element. (B) Freundlich adsorption isotherms for the enrichment of two analyte solutions.