

# A Versatile Porous Enrichment Layer for Monitoring Organic Contaminants in Water via ATR Spectroscopy

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With the growing awareness for environment and health as well as governmental regulations becoming stricter, there is an increasing need for fast and simple water monitoring technologies. Mid-IR spectroscopy is a powerful and well-established analytical method that provides access to the information-rich fingerprint region of the spectrum, which enables identification and quantification of organic contaminants. However, strong background absorption of water in the mid-IR region limits the technique's sensitivity. An increase in sensitivity is achieved by coating attenuated total reflectance (ATR) crystals or optical fibers with organic polymer coatings.[1,2,3] These coatings reversibly absorb and thereby concentrate the contaminant in the region probed by the evanescent wave, while excluding spectral interferences of the matrix water. Thereby limits of detection (LOD) for chlorinated and aromatic hydrocarbons in the mid-low ppb region have been reached. However, polymer coatings used in literature rely on long enrichment and recovery times due to the diffusion resistance of bulk polymers, which limits their practical applications for online monitoring. Diffusion and thereby response time can be enhanced by porous enrichment materials. In 1996 Lu et al. prepared porous sol-gel coatings of which enrichment times were at least 50 times faster compared to polymer coatings, but reached relatively low limits of detection (ca. 500 ppm). [4]

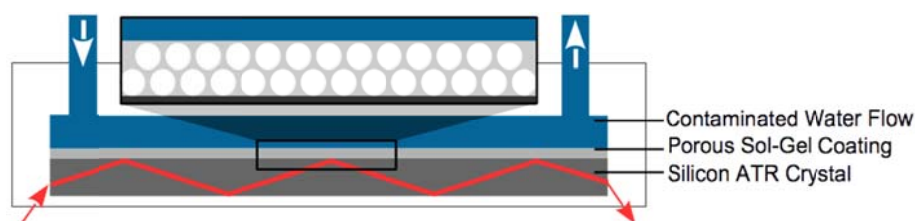


Figure 1: flow cell system with exchangeable ATR crystals coated with sol-gel materials.

Since then, sol-gel chemistry has enormously evolved and allows precise pore design and pore functionalization.[5] On this basis, we comprehensively studied the influence of chemical functionalization, pore size, pore shape and pore arrangement on the performance and enrichment times for the determination of hydrocarbons in water. Thereby LODs in the low ppm range were achieved while maintaining short response times (< 1 min). Alongside this study, we present a novel flow cell system with easily exchangeable ATR crystals from low-cost silicon wafers allowing for fast screening of an extensive series of enrichment layers.

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[2] Yang, J.; Cheng, M. L. et al. *Analyst* **2001**, *126* (6), 881–886.

[3] Göbel, R.; Krska, R.; Kellner, R.; Seitz, R. W.; Tomellini, S. A. *Appl. Spectrosc.* **1994**, *48* (6), 678–683.

[4] Lu, Y.; Han, L.; Brinker, J.; Niemczyk, T. M.; Lopez, G. P. *Sensors Actuators B* **1996**, *3536*, 517–521.

[5] Ciriminna, R.; Fidalgo, A.; Pandarus, V.; et al. *Chemical Reviews* **2013** *113* (8), 6592–6620.