Molecularly imprinted polymers are specialty polymers with ability of selectively capturing target molecules. They show great potential to be environmental sensors for the detection of specific contaminant. The overall research objective is to investigate the sensing ability of MIPs based on two mechanisms fluorescence quenching and reflectance for two example contaminants 2,4-dinitrotoluene and 2-butoxyethanol, which are fingerprinting contaminant of explosive manufacturing and hydraulic fracking. The water chemistry effects are explored on MIPs for their potential use as in-situ sensors in complex aquatic environments.

Fluorescent carbon dots with different surface functionality were fabricated and their environmental fate was explored. Amino-functionalized carbon dots (AC-dots) were applied to fluorescently label a molecularly imprinted polymer (MIP) for 2,4-dinitrotoluene (DNT) as a template. DNT is specifically captured by the cavities in the MIP and interact with AC-dots on the surface, resulting in quenching of the fluorescence of the AC-dots. Response to DNT reaches equilibrium within ~30 min. The method has a dynamic range that extends from 1 to 15 ppm, and allows for quantitation of DNT in aqueous solutions, with a detection limit of 0.28 ppm. Selectivity tests conducted in presence of DNT analogs demonstrated the specific recognition of DNT.

The effect of sample water chemistry on carbon dots labeled molecularly imprinted polymer (AC-MIP) sensor the detection of 2,4-dinitrotoluene (DNT) was investigated. With the increase of ionic strength from 1 mM to 100 mM, the quenching amount of MIPs decreased about 19% and 30% with NaCl and CaCl2 respectively. In the range of pH from 4 to 9, quenching effect is slightly higher at basic environment for both MIPs and non-imprinted polymers (NIPs) resulting from swelling properties of the films. NOM added the quenching amount to the sensor with a modified equation developed with NOM as a variable. In both lake water and tap water, DNT concentrations read by the sensors were very close to the HPLC measured DNT concentrations with the range from 72% to 105%.

Molecularly imprinted polymers (MIPs) sensors for detection of 2-butoxyethanol (2BE), a pollutant associated with hydraulic fracturing contamination, were developed based on the combination of a colloidal crystal templating method and a molecular imprinting technique. MIPs exhibited higher binding than non-imprinted films (NIPs) due to the specific adsorption provided by molecular imprinting with imprinting efficiencies around 2. Optical tests were performed because of the uniformly ordered porous structure. The reflectance spectra of the sensors showed Bragg’s peaks, which responded to the presence of 2BE; peaks presented increasing red shifts up to 50 nm with 2BE concentrations in the range of 1 ppb to 100 ppm, which allowed quantitative estimates of present 2BE concentration in aqueous solutions. The material has the potential for early detection of hydraulic fracturing sites contamination. The availability of early detection of hydraulic fracturing contamination is the main benefit to people and the planet from a human health perspective; secondly, and as a direct consequence of the former, the sustainable exploitation of a natural resource in the US and around the world has important implications for society development, economic growth and international relationships.