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## **ACCEPTED MANUSCRIPT**

#### Cyclodextrin-Functionalized Mesostructured Silica Nanoparticles for Removal of Polycyclic

#### **Aromatic Hydrocarbons**

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Abstract: Polycyclic aromatic hydrocarbons (PAHs) are the byproducts of the incomplete combustion of carbon-based fuels, and have high affinity towards DNA strands, ultimately exerting their carcinogenic effects. They are ubiquitous environmental contaminants, and can accumulate on tissues due to their lipophilic nature. In this article, we describe a novel concept for PAH removal from aqueous solutions using cyclodextrin-functionalized mesostructured silica nanoparticles (CDMSNs) and pristine mesostructured silica nanoparticles (MSNs). The adsorption applications of MSNs are greatly restricted due to the absence of surface functional groups on such particles. In this regard, cyclodextrins can serve as ideal functional molecules with their toroidal, cone-type structure, capable of inclusion-complex formation with many hydrophobic molecules, including genotoxic PAHs. The CDMSNs were synthesized by the surfactant-templated, NaOH-catalyzed condensation reactions of tetraethyl orthosilicate (TEOS) in the presence of two different types of cyclodextrin (i.e. hydroxypropyl- $\beta$ cyclodextrin (HP- $\beta$ -CD) and native  $\beta$ -cyclodextrin ( $\beta$ -CD)). The physical incorporation of CD moieties was supported by XPS, FT-IR, NMR, TGA and solid-state <sup>13</sup>C-NMR. The CDMSNs were treated with aqueous solutions of five different PAHs (e.g. pyrene, anthracene, phenanthrene, fluorene and fluoranthene). The functionalization of MSNs with cyclodextrin moieties significantly boosted the sorption capacity (q) of the MSNs up to ~2-fold, and the q ranged between 0.3 and 1.65 mg per gram CDMSNs, of which the performance was comparable to that of the activated carbon.

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