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Characterization and numerical investigation of 3D-printed porous organic cages for gas adsorption

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Porous organic cages (POCs) are a class of emerging microporous materials with high porosity and selectivity for gas adsorption and separation.[1] As a representative of first-generation POCs, CC3 has huge potential for separating noble gases and volatile organic compounds (VOCs).[2] Traditional manufacturing techniques exhibit some limitations in immobilizing the porous materials into structural adsorbents, such as poor transfer efficiency, insufficient loading of active material, limited structural forms, etc.[3] Three-dimensional (3D) printing demonstrates significant advantages in building complex structures with controlled features, to fully exploit their potential.[4] In this study, we demonstrate a versatile approach to 3D print porous materials, successfully shaping CC3 into hierarchically porous architectures by direct ink writing (DIW)[5]. Through the rational design of formulations, we obtained inks that combine both printability and functionality and printed a series of filter prototypes. The optimization of flow physics by tailoring the geometric parameters can effectively improve the contact, diffusion, mass transfer, and energy loss.[6] This is achieved by utilizing computational fluid dynamics (CFD) to numerically investigate the flow behavior and interactions through the structures for gas adsorption applications.[7]

The bentonite-based hybrid additive was used in the formulation as its unique layer structure constructs an interlinked network.[8] This brings the inks with good plasticity beneficial for printability and also retains active sites for CC3. The linear and nonlinear viscoelastic behavior of the inks with different CC3 loading (from 0wt% to 70wt%) were characterized by the oscillatory shear rheology to quantitatively study their printability. These inks were constructed into multiscale porous structures using DIW, and it was found that the crystal structure (Fig. 1a) and the adsorption capacity (Fig. 1b) of CC3 can be well preserved. The specific surface area is positively correlated with the loading amount of CC3, which can reach 249.35 m^2/g for 70wt% CC3 (Fig. 1b). However, the increase in CC3 content leads to a reduction in mechanical performance due to less shrinkage effect dominated by bentonite.[9]

Based on the printed structures (Fig. 1c and d), porous 2D repeating unit cells achieved with periodic boundary conditions with varying offset filament distance, pore size, and porosity were designed and simulated under different flow conditions using a commercial CFD package (Ansys Fluent). The extended Darcy-Brinkman-Forchheimer model was used to model the flow in the filament's porous zone.[10] The numerical results reveal that as the Reynolds number (Re) increases, a recirculation region develops and gradually expands within the gas flow path. Increasing offset distance brings more curved streamlines (Fig. 1e) and leads to a rise of pressure drop and overall flow resistance. The effect of filament's porosity and pore size on the pressure drop is investigated. This work provides a pathway for designing and fabricating high-performance adsorption systems, and can also be widely used for other functional materials for sustainable environment and energy applications.

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