Stability of MOF-5 in a hydrogen gas environment containing fueling station impurities - DTU Orbit (08/11/2017)

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Metal-organic frameworks (MOFs) are an emerging class of porous, crystalline materials with potential application as hydrogen storage media in fuel cell vehicles. Unlike lower capacity adsorbents such as zeolites and carbons, some MOFs are expected to degrade due to attack by impurities present in the hydrogen fuel stream. Hydrogen intended for use in fuel cell vehicles should satisfy purity standards, such as those outlined in SAE J2719. This standard limits the concentration of certain species in the fuel stream based primarily on their deleterious effects on PEM fuel cells. However, the impact of these contaminants on MOFs is mostly unknown. In the present study MOF-5 is adopted as a prototypical moisture-sensitive hydrogen storage material. Five “impure” gas mixtures were prepared by introducing low-to-moderate levels (i.e., up to ~200 times greater than the J2719 limit) of selected contaminants (NH_3, H_2S, HCl, H_2O, CO, CO_2, CH_4, O_2, N_2, and He) to pure hydrogen gas. Subsequently, MOF-5 was exposed to these mixtures over hundreds of adsorption/desorption pressure-swing cycles and for extended periods of static exposure. The impact of exposure was assessed by periodically measuring the hydrogen storage capacity of an exposed sample. Hydrogen chloride was observed to be the only impurity that yielded a measurable, albeit small, decrease in hydrogen capacity; no change in H2 uptake was observed for the other impurities. Post-cycling and post-storage MOF-5 samples were also analyzed using infrared spectroscopy and x-ray diffraction. These analyses reveal slight changes in the spectra for those samples exposed to HCl and NH3 compared to the pristine material. These measurements suggest that MOF-5 – and likely many other MOFs – exhibit sufficient robustness to withstand prolonged exposure to ‘off-spec’ hydrogen fuel.

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