Functionalization of Nanoporous Carbons for Hydrogen Storage

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Motivation

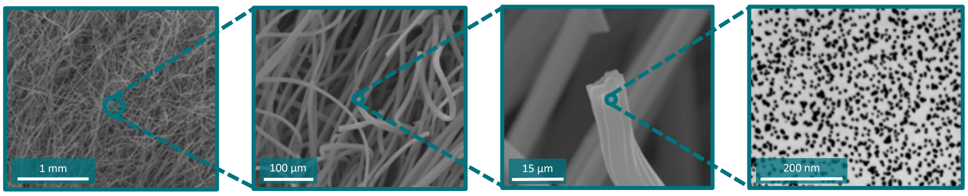
A climate-neutral Europe requires
- large-scale **hydrogen production** and
- efficient hydrogen **storage capacities.**

We investigated a novel hydrogen storage approach by developing a composite material consisting of
- **Activated carbon cloth** (highly porous, surface area of 1820 m²/g)
- **Metal nanoparticles** (NPs) for catalyzing hydrogen adsorption

Material System

Within this work, we attempt to store hydrogen on the surface of **nanoporous carbons**.

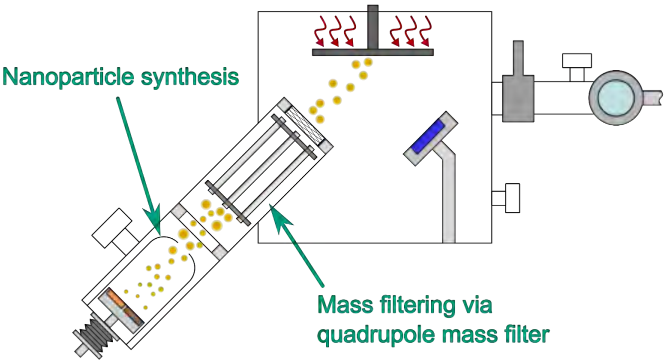
The carbonaceous surface is **functionalized** using metal nanoparticles (diameter: 2 nm … 10 nm) to enhance to hydrogen uptake at room temperature (**hydrogen spillover effect**).



Nanoparticle Synthesis

Magnetron Sputter Inert Gas Condensation is used for nanoparticle synthesis.

A schematic of the used nanoparticle deposition system consisting of the nanoparticle source and the deposition chamber is given below:

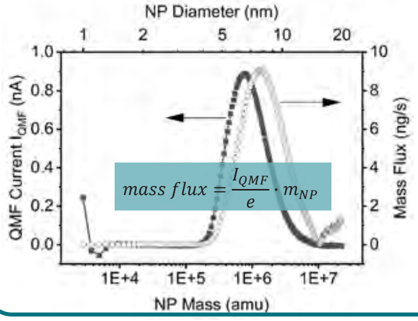


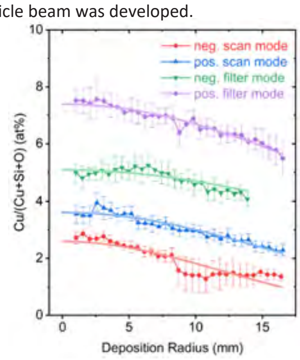
<u>Synthesis steps:</u>
1. Metal atoms are ejected from the metal target in a sputter process.
2. Atoms condense to metal nanoparticles within a high-pressure chamber filled with inert gases (e.g. Ar, He).
3. Fully developed nanoparticles may be mass-filtered using a quadrupole mass filter within a low-pressure zone.
4. The nanoparticle beam terminates at the substrate.

Quantifying Nanoparticles

A method for ***in-situ*** **characterization** of the nanoparticle beam was developed.

The **mass flux** of the nanoparticle beam can be **calculated** by using the current measured via the quadrupole mass filter (I_{QMF}), the nanoparticle mass m_{NP} and the elementary charge e.

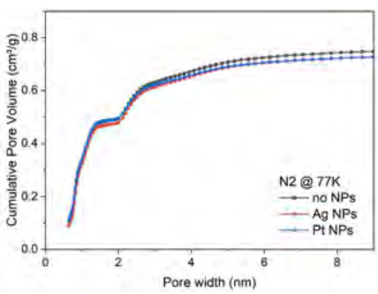




X-ray photoelectron spectroscopy confirmed the **Gaussian distribution** of the **spatial arrangement** of the nanoparticles after deposition.

Pore Structure

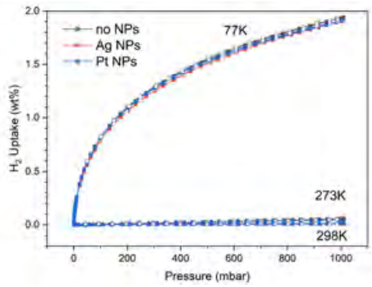
The pore structure was investigated via gas sorption analysis using N_2 **@ 77 K** from 0 to 1 bar.



- The cumulative pore volume is slightly larger for the pristine sample.
- This indicates **minor pore blocking** caused by the deposited metal nanoparticles.
- Complementary characterization via Raman spectroscopy and X-ray diffraction revealed **no structural changes** caused by the nanoparticle deposition.

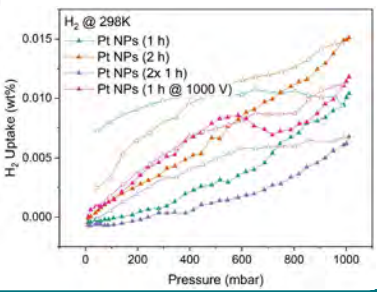
Hydrogen Storage Performance

Gas sorption analysis was performed using H_2 **from 0 to 1 bar** in order to assess the hydrogen storage performance at various temperatures.



- At low temperatures (77 K), hydrogen adsorption occurs proportionally to the specific surface area.
- The **pristine carbon cloth** showed the **highest storage capacity at low temperatures** as it had a slightly higher specific surface area.
- At higher temperatures (273K, 298K) hydrogen uptake is reduced drastically.

- Multiple samples were prepared using different synthesis conditions and deposition times.
- The **highest hydrogen uptake (0.015 wt%)** was observed after depositing Pt nanoparticles for 2 h (mass-filtered nanoparticles with a diameter of 4 nm).
- **No** indication of the **hydrogen spillover** effect could be confirmed up to now.



Conclusions

Magnetron sputter inert gas condensation was **successfully established** as a process for **nanoparticle synthesis**.

An ***in-situ*** **characterization method** for quantifying the nanoparticle beam based on quadrupole mass spectrometry was **successfully developed and implemented**.

Functionalized activated carbon cloths decorated with Pt nanoparticles were synthesized and showed **poor hydrogen storage performance (< 0.015 wt%)** at **room temperature**.

Manuscript under preparation: Knabl F.; Bandl C.; Grießer T.; Mitterer C.; *"A novel method for quantification of nanoparticle fluxes in magnetron sputter inert gas condensation."*

To enhance hydrogen storage performance, we will explore potential solutions:
- **Improved nanoparticle dispersion** on a three-dimensional substrate by performing depositions under substrate bias.
- **Improved total nanoparticle output** from the nanoparticle source (e.g. addition of oxygen to the inert gas flow)

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