



Biomass-derived Activated Carbon for H₂ storage: influence of solvent and doping agent on the adsorption properties

Alessia MARINO¹, Carlo POSELLE BONAVENTURA², Sara SCIARRETTA¹, Giuseppe CONTE², Alfredo ALOISE¹, Chiara PELOSI³, Andrea LAZZARINI¹, Celia DUCE³, Luca BERNAZZANI³, Alfonso POLICICCHIO², Marcello CRUCIANELLI¹

¹ University of L'Aquila, Department of Physical and Chemical Sciences, via Vetoio, 67100, L'Aquila, Italy.

² University of Calabria, Physics Department, Via Bucci, 87036, Rende, Cosenza, Italy.

³ University of Pisa, Department of Chemistry and industrial chemistry, Via Moruzzi, 56124, Pisa, Italy.

alessia.marino3@univaq.it

Significance and Relevance

Hydrogen represents a suitable alternative to fossil fuels, but efficient storage is still challenging. Biomass-derived carbons, enhanced by heteroatom doping, offer a promising solution. This work investigates boron-doped activated carbons for H₂ storage, by evaluating the impact of solvents and reaction conditions on textural properties and adsorption performance. Results show that both reaction time and solvent type affect surface area, and then the hydrogen adsorption, indicating that the presence of boron can improve H₂ uptake at 77 K, while harsh reaction conditions may cause a structural collapse.

Preferred and 2nd choice for the topic: "H₂ storage and transportation, green H₂ production, hydrogen vectors", and "Sustainable and clean energy production and transport"

Preferred presentation: Oral preferred or Short Oral

Introduction and Motivations

In the view of reaching the carbon neutrality, new solutions for energy production and transportation are matter of studies from the scientific community. In this context, hydrogen represents one of the most promising clean and sustainable alternative to fossil fuels. However, the limiting factor still lies in its storage, since it requires both an efficient adsorption and a highly reversible release under mild conditions. Biomass-derived carbons represent a class of efficient and low-cost materials suitable to this purpose, which can be further upgraded by adjusting textural properties, as well as by inserting heteroatoms as dopant [1]. In this work, the influence of boron as activated carbon-dopant on the H₂ adsorption-desorption properties has been studied [2]. To this aim, the role of different solvents and times, generally used in boronation reactions, was also investigated, in order to correlate the change in the textural properties and the actual contribution of the selected heteroatom [3].

Materials and Methods

Coconut-derived activated carbon was added to the selected solvent and then the mixture was kept under stirring for designated times (3, 7, or 10 days) at 80 °C. The solid was then separated by centrifugation and dried. The solvent-carbon matrix interaction has been investigated for the following solvents: tetrahydrofuran, N-methyl-2-pyrrolidone, 1,2-dimethoxyethane, toluene, deionized water, ethanol, and isopropyl alcohol. A similar procedure was used for boron doping, by adding to the mixture different concentrations of BH₃ (8 and 17 mmol/g). The obtained samples were characterised by N₂-physisorption, TGA-IR, Raman and IR spectroscopy, and SEM. The H₂ storage performance was evaluated at low pressure (up to 1 bar).

Results and Discussion

The solvents screening has evidenced a general change in the textural and morphological (**Figure 1**) properties of the activated carbon, as a function of both solvent type and reaction time, regardless the presence of the doping agent.

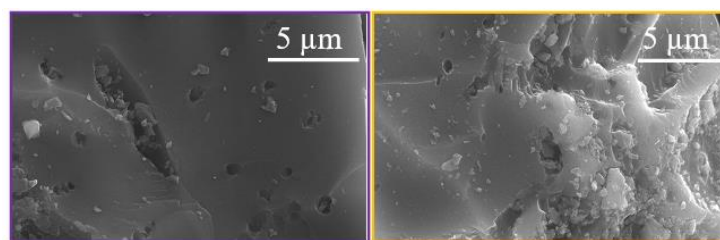


Figure 1 – SEM images of parent activated carbon (left, purple) and after treatment in THF for 10 days (right, yellow).

In particular, NMP_7d and TOL_3d showed the highest surface area decrease, while just a small modification was observed in THF_3d, compared to the parent carbon. As expected, these results reflect on H_2 storage performance, showing that the adsorption is strictly related to the available surface area. When boron was used as doping agent, two different effects were observed as a function of borane concentration and reaction time. In particular, the H_2 uptake increased according to the reaction time when the lowest concentration of BH_3 was used, while by doubling the amount of B the opposite trend was observed (**Figure 2**). Lastly, both the highest concentrations of dopant boron and times led to a collapse of the activated carbon framework.

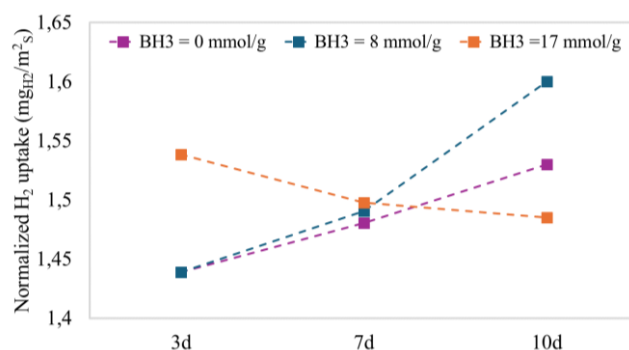


Figure 2 – Normalized H_2 uptake vs time and BH_3 concentration.

The obtained results revealed an active role of solvent and reaction time on the activated carbons framework modification, which impacts the H_2 storage performance. However, the presence of B can improve H_2 adsorption-desorption properties, despite the solvent-related effects, demonstrating the high potential of these doped biomass-derived carbons in H_2 storage application.

References

1. A. Lazzarini et al., *Compounds*, **2023**, 3(1).
2. A. Marino et al., "Evaluation of solvent role in biomass-derived activated carbon functionalization for H_2 storage", in preparation.
3. A. Marino et al., "Boronation of biomass-derived activated carbon for H_2 storage application", in preparation.