

1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan)

Project title: Designing the novel nanomaterials for hydrogen storage

1.1. Project goals

The main objective of the project is the design of highly effective, novel materials for hydrogen storage. The main question to answer is how to design carbon-based nanocomposites to work as active and stable adsorbents for hydrogen. We would also like to explore the role of nitrogen heteroatoms incorporated into the carbon matrix and the role of porosity on storage efficiency.

The particular goals:

- Designing the adsorbents - synthesis and full physicochemical characterization of C-based composites using adsorptive and spectroscopic techniques
- Adsorption conditions optimization
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- Tackling Climate Change, our duty is to contribute to lowering greenhouse gas emissions and delaying climate change.
- Energy Security: It can help improve energy security by reducing reliance on imported fossil fuels.
- Job Creation: Jobs can be created by developing and implementing sustainable fuels and chemical production technologies.
- Economic Growth: It can open up new business opportunities and promote economic expansion.
- Environmental advantages: The proposed study can support the advancement of environmentally friendly business practices and lessen the environmental impact of diverse businesses.

1.2. Outline

Hydrogen energy and storage are gaining significant attention due to their potential to address various energy and environmental challenges. The storage of hydrogen in solid-state media is an area of significant interest and research in comparison to compressed gas or liquefied hydrogen storage in high-pressure and large-volume storage tanks. Solid materials can store hydrogen in a condensed form, allowing more hydrogen to be stored within a smaller volume or mass. In addition, solid-state materials offer safer hydrogen storage compared to gaseous or liquid hydrogen where hydrogen is stored at very high pressure (350–700 bar). Extensive research has been carried out on graphene-based materials doped with heteroatoms, showing promise as potential candidates for hydrogen storage. This is attributed to their distinctive properties and improved ability to adsorb hydrogen. Several heteroatoms, such as nitrogen, boron, and sulfur, have been extensively studied for their effects on graphene's hydrogen storage performance.

1.3. Work plan

1. **Carbon-matrices synthesis. (i) amorphous carbons (based on biocarbons), (ii) Graphene oxide, (iii) reduced graphene oxide, and composites**
2. **Nitrogen-doping.** Various amount of doped nitrogen will be introduced to carbon materials to investigate its effects on the catalytic efficiency.
3. **Nanocomposites synthesis.** The hybrids of the C-matrix and single- bi-, and tri-metallic systems deposited on carbons will be synthesized.
4. **Porosity measurements.** The low-temperature nitrogen adsorption measurements: surface area and volume; H₂O, NH₃, CO₂ will also be used as adsorbate to characterize the material.
5. **Full phys-chem characterization;** all available techniques will be used:
 - SEM/EDS: the size, shape, surface texture and morphology of the crystals, and chemical composition;
 - HRTEM/EDX: the pore size, internal structure and morphology of crystals, helps to analyze the chemical composition of materials;
 - TG: thermal stability of prepared nanomaterials; this technique is a good method to check whether the MOF has been sufficiently activated (no residual solvent molecules);
 - PXRD: the crystal structure, phase composition;
 - Sorption of NH₃, CO₂ and H₂O combined with spectral studies - determination of chemical properties and mechanism of splitting; for the in situ IR study the pelletized samples will be exposed to target gas.
 - Additionally, the obtained materials will be fully characterized spectroscopically: XPS, IR, RS.

6. Finally, the adsorption process of H₂ storage will be evaluated. The collected results will be enriched by in-situ FTIR measurements.

7. The results are expected to be published in high-impact-factor scientific journal.

- The results obtained during the project realization
 - Activity and selectivity of newly synthesized materials
 - Description the process mechanismwill be published in high-impact-factor scientific journal

1.4. Literature (max. 7 listed, as a suggestion for a PhD candidate preliminary study)

1. Ghotia et al, *J Mat Chem A*, 2024, DOI: 10.1039/d4ta00717d
2. Liu et al, *Batt Energy*, 2022, DOI: 10.1002/bte2.20220033

1.5. Required initial knowledge and skills of the PhD candidate

- knowledge on chemistry
- basic understanding of catalysis
- understanding of chemical and material's characterization techniques
- analytical thinking and skills
- open to challenging tasks and creative
- hard-working person, eager to learn

1.6. Expected development of the PhD candidate's knowledge and skills

- ability to plan and organize laboratory work
- skilled in novel scientific techniques
- ability to solve research problems
- innovative thinking
- ready to work in an international research group