

Olefins (unsaturated hydrocarbons, alkenes), in particular ethylene and propylene, are vital building blocks of polymers and plastics. The global production of olefins exceeds 300 million tonnes annually (roughly 35 kg per living person), with the prediction to increase. The typical olefins production process (steam cracking of naphtha) is extremely energy intensive, emissive, and mostly fueled by non-renewable energy sources. For example, the estimated annual energy demand for production of ethylene (3.5 EJ) is similar to the total energy consumption of Kazakhstan (3.7 EJ). Due to the large volume production of olefins even small improvements in the process efficiency offers large rewards to the sustainability, which is crucial for the transition towards the net-zero-greenhouse emissions economy.

Apart from ethylene and propylene, steam cracking products contains corresponding paraffins (saturated hydrocarbons), other olefins and aromatic hydrocarbons. Owing to the low boiling point and very similar physicochemical properties, polymer grade olefins are separated from their respective paraffins in the train of cryogenic distillation columns operating under extreme conditions (low temperature, high pressure). Despite the maturity, the distillation suffers from the low thermodynamic efficiency and high energy consumption. Finding an efficient alternative could reduce the energy intensity of the olefin production by several orders of magnitude.

The adsorption, *i.e.*, adherence and accumulation of molecules onto a solid surface (adsorbent), can be a feasible separation strategy, provided that highly selective adsorbents can be engineered. Adsorptive separations have wide application due to several advantages, *e.g.*, energy efficiency, simple design, ease of operation and maintenance, or flexibility. However, despite over 40 years of research on different types of adsorbent, no practical solution to the paraffin/olefin separation problem was proposed. Nevertheless, the search for selective adsorbents continues, because of the high reward to risk ratio. Recently, aerogels made of reduced graphene oxide (rGO) have emerged as technology enhancing materials capable of connecting unique 2D properties of the graphene with practical 3D objects, also in the field of adsorption.

Reduced graphene oxide aerogels (rGOAs) are obtained by the sol-gel method from the graphene oxide (GO) dispersion, followed by the freeze- or supercritical-drying. The rGOA structure is composed of closely stacked and partially overlapping rGO flakes, which can have random or oriented arrangement, resulting in the hierarchical mesoporosity and wrinkled texture. The surface area of rGOAs can range between tens to few hundreds m^2/g . Chemistry of the rGOAs surface is dominated by delocalized π -electrons, defects in the hexagonal ring structure, and residual oxygen functional groups. Therefore, the surface can interact in different ways with adsorbates including van der Waals, hydrophobic, electrostatic, hydrogen bonds or ion- π interactions.

Although few reports about the gas phase adsorption on rGOA are available, we hypothesize that highly interconnected porous structure and the π -electron-rich surface can be of high importance for the adsorption of olefins and paraffins, and will enable selective adsorption based on the difference in olefin/paraffin – rGOA surface strength of interactions (thermodynamic mechanism) and difference in the kinetic diameter of molecules (kinetic mechanism). Therefore project aims at addressing the following questions:

1. To what extent pristine rGOAs can adsorb olefins and paraffins, and how it is related to the physicochemical structure of aerogels?
2. How the structure of an olefin affect the interaction with rGOAs, compared to a corresponding paraffin?
3. Is the difference between olefins and paraffins adsorption big enough to call pristine rGOAs a selective adsorbent?
4. To what extent competitive adsorption is compromising separation efficiency?
5. Is there a room for improvement in terms of selectivity and capacity of rGOAs?

In the course of the project a number of aerogels will be synthesized and comprehensively characterized with the state-of-the-art methods. Results of the adsorption test with different olefin and paraffin probe compounds, in single and binary systems, will be correlated with aerogels and olefins structure to reveal mechanisms of the adsorption.

The pioneering nature of the project urges us to put emphasis on producing high quality data that will go beyond the current knowledge, and provide foundation for further research, both basic and applied. Hopefully, we will be able to provide fundamental mechanistic insights on the rational design and engineering of rGOAs that will eventually force other research areas beyond adsorption, such as catalysis, energy storage, sensors or polymer additives.