Environmental changes, as well as environmental regulations, contributed to change in the energy sector. The accessibility of solar and wind energy-harvesting technologies are constantly increasing, opening a challenge for developing efficient and economical energy storage solutions that need to solve the problem of the intermittent nature of renewable energy. Phase-change materials (PCM) that are capable to store or release energy during the phase transition, preferably melting and crystallization can become of key importance for sustainable and economical wide-scale renewable energy storage.

PCMs that melt in the intermediate temperature range (100-220 ºC) have been recently recognized as promising for renewable energy storage in the thermal battery application (Carnot Battery). This technology has potential to change the renewable energy storage market as it is inexpensive and easily scalable. Moreover, the adoption of this technology on the large scale, will significantly reduce the amount of fossil fuels used to generate electricity, contributing to substantial saving of CO_2 emissions. Nevertheless, the cost, efficiency and sustainability of this technology are critically dependent on the origin, performance, and price of the PCMs involved. While PCMs, as a general concept are well known, the choice of existing materials with melting points in the 100- 220°C range (suitable for this application), which additionally meet the sustainability and circularity criteria is limited.

Among organic materials that melt in the desired temperature range naturally occurring sugar alcohols and their derivatives possess the highest enthalpy of fusion. Although these materials are non-toxic, non-flammable, non-corrosive and most of all fulfill the criteria of materials circularity, key to our transition to net-zero, they suffer from low cycling stability (repetitive melting and crystallization) and large supercooling (temperature difference between a material's melting point (T_m) and the temperature at which it regularly crystallizes (T_c), what excludes them from the use as PCMs in the pure form.

Our recent results show that transforming sugars into salts can significantly reduce supercooling in polyol phase change materials and increase their stability by introducing additional Coulombic interactions. Moreover, our studies performed with the researchers from Monash University (Australia) reveal that introducing additional van der Waals forces substantially contribute to improvement of the thermal properties of polyol PCMs.

Under this project sugar alcohols/acids will be converted into organic salts/ionic liquids, amide/urethane/urea derivatives with additional Coulombic/Van der Waals interactions to finely tune and improve their thermophysical properties. The project aims to determine and understand the molecular interactions in the new materials in the solid state and during the phase transition and to correlate these interactions with their fundamental thermal properties. These determined structure-property relationships will contribute to the development of sustainable materials with enhanced properties for efficient and sustainable heat use.

The study will involve the design of new materials, and elaboration of the most promising synthetic routes and reaction conditions for their synthesis, according to the Principles of Green Chemistry. The developed materials will be further studied in terms of their thermophysical properties (using differential scanning calorimetry and thermal gravimetric analysis) and molecular interactions (using single crystal X-ray crystallography and Hirshfeld surface analysis). Compounds with the most promising thermal properties will be further tested for their long term stability and cyclability. A comprehensive grasp of the structure-function relationships in materials derived from biorenewable precursors will offer valuable insights, guiding the future design of sustainable phase change materials.