Catch the Heat!

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In order to tackle the modern challenges of climate change, resources depletion and geopolitical instability, the human society will have to evolve towards sustainable energy and green economy. Energy storage will play a paramount role in this global energy system, in order to support the penetration of the fluctuating renewable energy sources (sun, wind), as well as to capture the waste from various domestic or industrial processes.

As of 2022 **heat is the world's largest energy end-use**, accounting for ~50% of the world energy consumption (more than electricity - 30% or transport - 20%). About half of this heat is used in domestic applications, with the other half being used in industry. Creating efficient heat batteries able to store renewable and waste heat from natural (Sun) or artificial (industry) sources, at various temperatures, will be crucial for the implementation of the sustainable energy systems of the future.

Thermochemical energy storage (TCES) through reversible chemical reactions (sorption/desorption of gases like H_2O or CO_2) is the most promising technology for compact and lossless long-term heat storage. The current research in this field is hampered by the scarcity of appropriate TCES materials that can store and release heat at the desired temperatures with high efficiency and storage density. Thus, novel promising candidates are required, along with means of screening the large potential chemistry structural space.

In our work we performed a high-throughput screening of structural databases (COD, ICSD) and by using a combination between machine learning, advance chemical reactivity descriptors and DFT-calculations we established ML-based structure-thermodynamics descriptors that are able to predict thermodynamic characteristics (enthalpy/entropy of reaction) for two classes of materials relevant for heat storage at low and high temperatures: salt hydrates and metal oxides. Having as basis the computational results obtained, we initiated the first open comprehensive database of thermochemical materials (**tess-db.com**, recently launched), in order to provide a toolkit to assist researchers and engineers in materials discovery and creation of new energy storage devices. The platform is intended to create an open bridge between material scientists, engineers and policymakers in the field of thermal energy storage, in order to share data and tackle collaboratively society challenges. It is also intended to support related fields, such as thermochemical water splitting or carbon capture and storage, where the interaction between a gas (like H_2O or CO_2) and a bulk material (like oxide or salt) it is of relevance.