ChemAppPy Friendly Case Studies: A journey through accelerated large-scale thermochemical investigations

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It is often challenging and time-consuming to conduct large-scale thermochemical investigations. This is mainly due to the numerous thermochemical calculations required and subsequent data analysis involved to clearly understand the problem. Often multiple investigations are required to come to a clear understanding of the thermochemical behaviour. Ex Mente developed ChemAppPy Friendly, a software tool that combines FactSage data, the power of ChemApp, and the flexibility and freedom of Python and other open-source software into a friendly environment to conduct such large-scale investigations rapidly and effectively.

We will present why ChemAppPy Friendly was developed and give an overview of how the different tools such as FactSage and ChemApp fit into the picture. We will also give a brief explanation of how ChemAppPy Friendly can be used. Different industrial case studies in which the tools were used will be discussed. The benefits of the software will also be explained and demonstrated.