

## Scanning chemical compound space for radically new processing solutions: de-bismuthizing lead

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Many metallurgical processes rely on recipes that have been developed over decades based on empirical research. This talk will propose a way to identify possible radically new processing solutions based on thermochemical data.

As an example, de-bismuthizing of lead is discussed which is one of the final stages of lead refining. The Kroll-Betterton process was developed in the 1930s and is still used today. To remove bismuth from the lead melt, Ca and Mg are added to form  $Mg_2CaBi_2$  which floats on the melt and can be separated. This process is very time-consuming, expensive and rather inefficient (a significant amount of lead is lost together with the solid particles). However, it is still the best process known to date!

Using the new database aiMP (ab initio materialsproject) together with the SGTE Solutions database, whole chemical compound space is scanned for alternative process solutions. 53 binary additions to Pb-Bi are identified that result in an equally low or lower Bi content as  $Mg_2Ca$ . Thus, trends in chemical compound space can be identified and the number of experiments needed to identify best additions can be drastically reduced.