

## **Looking for future solutions by digging into the past: How computational thermochemistry can help us solve old industrial mysteries.**

*Authors: Sabine Khadhraoui <sup>1)</sup>, Klaus Hack <sup>2)</sup>, Tatjana Jantzen <sup>2)</sup>*

*<sup>1)</sup> SMS group GmbH, Germany <sup>2)</sup> GTT Technologies, Germany*

Metallurgy is an old science, which has been established over few millennia. Despite the huge developments achieved in modern steelmaking, several aspects remain unclear. This includes the thermodynamics and kinetics of important metal-slag-gas reactions, such as dephosphorization.

Today, modern computational methods developed in the field of materials science such as computational thermochemistry, provide us with a powerful instrument, which we can use to evaluate and optimize metallurgical processes. It is now possible to re-evaluate a large amount of old industrial data using computational thermochemistry, in the hope of gaining new information, which can help us optimize current industrial practices. That is, by digging into the past we may be able to improve the present and the future of steelmaking processes.

In this talk, some examples of old industrial controversies related to the thermodynamics of dephosphorization reported back in the 1960s are brought up and discussed. The controversies are re-investigated using computational thermodynamics approaches, which were not available back then. The relevance of those findings for improving dephosphorization in modern steelmaking processes is discussed.