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The Sapiens project: a call for creating sustainable thermodynamic databases

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Probably CALPHAD databases users most frequent questions are: What is the origin of the information? Which data is inside? Can they be updated using my new experimental data? Can I change the model? How to connect them to 0 K first-principles calculated quantities? How to extract stable and metastable information to use in my own code for microstructure simulations?

Some of these questions are difficult to be answered even by CALPHAD databases creators. Changes, for example, in the melting temperature of a single pure element have an impact in the multicomponent database that is not easy to be evaluated if the model parameters and their relationship are not well documented. Proposals for changes to more physical models are available in literature since long time (see by instance the Ringberg series of recommendations sponsored by SGTE and Max-Planck Society), however, they have not been implemented even by SGTE due to the immense work it would require.

Motivate by these questions, the Sapiens project is created proposing well documented, flexible, cooperative and open work for the construction of knowledge-based and sustainable thermodynamic databases. Steels are selected as starting materials due to their challenging complexity which motivates several theoretical fronts in materials science like magnetism and metastability.

Sapiens project collects experimental data and uses physical based models at their best providing a forum for discussions and tests of new models and different applications. Iron and Chromium are the first elements studied in the project and first results are presented in this conference. Sapiens has industrial support and is purely academic. A call for international cooperation is done.