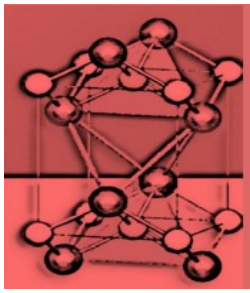

XI Workshop on Novel Methods for Electronic Structure Calculations

16th – 17th December 2024

La Plata – Argentina

How the Effective Bond Energy Formalism (EBEF) benefits from first-principles results

Silvana Tumminello [a], Suzana G. Fries [b]

[a] *Institute of Materials Research, German Aerospace Center (DLR), Cologne, Germany.*

[b] *Materials Research Department, Ruhr University Bochum (RUB), Bochum, Germany.*

email:

Materials development and implementation relies nowadays on multiscale computational simulations to efficiently design the experimental steps of materials/components from their production and life-cycle to their reuse or recycle [1,2].

In the mesoscale range, materials simulations make intensive use of calculated phase diagrams and thermodynamic properties with commercial and open-source thermodynamic software and encoded thermodynamic information developed with the CALPHAD method (Calculation of Phase Diagrams and Thermochemistry) [3]. The strength of this method is the excellent ability to make reliable extrapolations in temperatures and compositions within the accuracy of experimental measurements. Several models are used to describe all the stable and metastable phases in a given material system, most of them are based on the Compound Energy Formalism that can greatly benefit from electronic methods, such as DFT (Density Functional Theory), incorporating energies of hypothetical compounds (end-members). The Effective Bond Energy Formalism is a recently developed method [4,5,6] which benefits from DFT calculated end-members to obtain effective bonding energies, and in this way, improving the extrapolation behavior in high-order material systems and reducing model parameters achieving lower computational effort and time.

We present examples of significant technological interest, sigma and mu phase in steel, Ni-based and Co-based superalloys, where EBEF has been tested and validated against experimental measurements, software where this method is already implemented and potential application cases.

[1]. S. Tumminello, et al., "Applications of thermodynamic calculations to practical TEG design: $Mg_2(Si_{0.3}Sn_{0.7})$/Cu interconnections," Journal of Materials Chemistry A, 9:36 (2021) 20436–20452. doi: 10.1039/D1TA05289F.

[2]. S. Tumminello et al., "DFT-CEF Approach for the Thermodynamic Properties and Volume of Stable and Metastable Al–Ni Compounds," Metals, 10: 9 (2020) 1142. doi: 10.3390/met10091142.

[3]. H. Lukas, S. G. Fries, and B. Sundman, Computational Thermodynamics. The Calphad Method. Cambridge University Press, (2007).

[4]. Dupin N, Kattner UR, Sundman B, Palumbo M, Fries SG, "Implementation of an Effective Bond Energy Formalism in the Multicomponent Calphad Approach". J Res Natl Inst Stan, 23 (2018) 123020. https://doi.org/10.6028/jres.123.020.

[5]. J. Pereira dos Santos et al. "Applying the Effective Bond Energy Formalism (EBEF) to Describe (σ) the Sigma Phase in the Co-Cr-Ni-Re System", J. Phase Equilib. Diffus. (2023). https://doi.org/10.1007//s11669-023-01079-3

[6]. Dupin N, "The Effective Bond Energy Formalism", TofA Meeting 2024.