

# Thermodynamic assessment of the Co–Mg system supported by ab-initio calculations

*N. Djenane and Y. Djaballah*

Laboratoire d'études Physico-Chimiques des Matériaux (LEPCM),  
Département de Physique, Faculté des Sciences de la Matière, Université de  
Batna 1

[n.djenane@yahoo.fr](mailto:n.djenane@yahoo.fr)

## Abstract

The objective of this work is the thermodynamic modeling of the Co-Mg binary system using two methods: The CALPHAD method (Calculation of Phase diagrams) and the ab-initio calculations.

CALPHAD is a very important method for modeling thermodynamic properties of phase diagrams for systems with several components. This method is based on a semi approach by modeling the free energies of the different phases existing in a system. Therefore reliable experimental data are necessary for the description of thermodynamic properties of phases. The basic principles of this method are to harmonize a set of this experimental and theoretical information. The theoretical thermodynamic data are obtained by the ab-initio calculation. The enthalpies of formation of defined compounds are obtained by a calculation based on the first principle quantum simulations also called ab-initio method that allow the theoretical determination of various properties (electronic, structural, energy, etc .. ) of the material without using experimental tools.

The phase diagram of the Co-Mg system has a single defined compound which is  $\text{Co}_2\text{Mg}$ . its enthalpy of formation is calculated using the WIEN2k code based on the method "full-potential linearized augmented plane-wave" and the GGA approximation "Generalized gradient approximation". The liquid phase was modeled using the Redlich-Kister polynomial. The results obtained are in good agreement with experimental results.

**Keywords:** Phase diagram, Co-Mg system, thermodynamic assessments, Calphad, Ab-initio calculations