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SESSION 1: MODELS AND METHODS, SALON A

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Calculation of thermodynamic and physical properties in multi-component systems

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ABSTRACT

Thermodynamic and physical properties are important for understanding other materials properties. Calculations of various properties, such as activity, partial pressure, and density, will be presented. Calculation is based on CALPHAD approach. A property could be calculated as a function of one variable (1D calculation) or as a function of two variables (2D contour diagram). Optimal property in a multi-component system could be searched by the brute-force method or other optimization algorithms.

KEYWORDS: thermodynamic properties, physical properties, CALPHAD, contour diagram