

THE FORMATION ENTHALPIES OF INTERMETALLIC COMPOUNDS IN SYSTEMS (Ni,Pd,Pt)–(Al,In,Sn) BY pySIPFENN SOFTWARE TOOL

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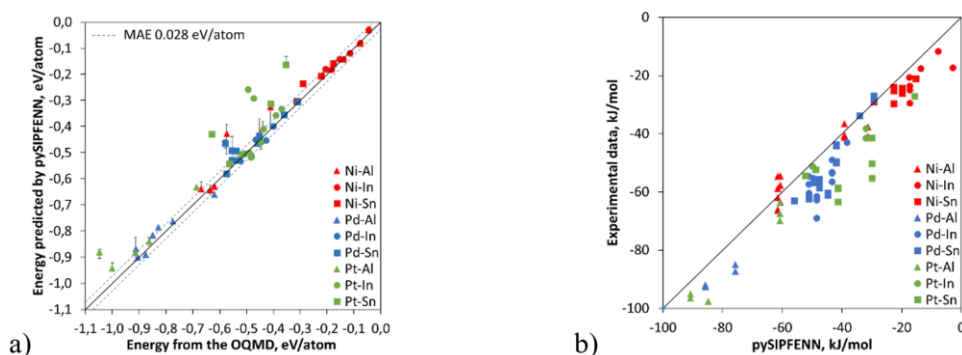
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First-principles calculations based on density functional theory (DFT) serve as an important source of input data for calculations using the CALPHAD method. They not only complement experimental results for stable phases but also provide data on metastable and virtual phases required for such calculations.

DFT calculations are resource-intensive and complex, so deep neural network (DNN) models have been increasingly used in recent years to determine formation energies. An example of a DNN-based tool is pySIPFENN [1].

The performance of pySIPFENN was assessed for the calculation of formation enthalpies of the compounds formed by transition metals from 10th group with *p*-metals from groups 13 and 14. Published structural data in the CIF format were used as initial data. In Figure 1(a), the calculation results are compared with OQMD data [2], while Figure 1(b) presents a comparison with available experimental values. In most cases, the pySIPFENN results agree with DFT calculations within the mean absolute error (MAE) of 0.028 eV/atom declared by the pySIPFENN developers. For two isostructural compounds, Pd₈Al₂₁ and Pt₈Al₂₁, unsatisfactory results were obtained. A comparison with experimental data reveals that pySIPFENN predictions exhibit a systematic shift of approximately 0.073 eV/atom (~7 kJ/mol) and a root-mean-square deviation of 0.092 eV/atom (~9 kJ/mol). This accuracy is sufficient to use pySIPFENN for estimating formation enthalpies of phases or end-members.



Comparison of pySIPFENN forecast results with (a) OQMD and (b) experimental data

1. Krajewski A. M. et al. // Computational Materials Science. 2022. Vol. 208, Nr 111254. <https://doi.org/10.1016/j.commatsci.2022.111254>

2. Saal J. E. et al. // JOM. 2013. Vol. 65, Nr 11. P. 1501–1509

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