

Supplementary information

Ultra-High-Entropy Alloy Nanoparticles: Beyond Five Components

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Code instructions

The code used to calculate the free energy, mixing enthalpy databases, mixing entropy, and delta parameters of the multi-element alloys is available at <https://github.com/julien-mahin/HEANPcalculator.git>. The data repository includes binary enthalpy databases based on Takeuchi *et al.* and Troparevsky *et al.*, dependencies, and instructions for reproducing the results. The provided Python script implements a graphical user interface (GUI) to calculate the free energy of multi-element alloys. The program allows users to select elements from the periodic table, input atomic percentages, and specify a reaction temperature. It calculates the following properties: Mixing Enthalpy: Based on binary enthalpy databases (Takeuchi and Troparevsky), Mixing Entropy: Using the ideal entropy of mixing formula, Delta Parameter: A measure of atomic size mismatch., Free Energy: Calculated as a function of enthalpy, entropy, and temperature. The GUI was built using the tkinter library, and the calculations rely on pandas and numpy for data handling and numerical operations.

Table S1: Various publications and HEANPs reviewed in this work, as well as the reaction conditions, calculated values for the mixing entropy, mixing enthalpy (based on either the data from Takeuchi *et al.* or Troparevsky *et al.*), corresponding mixing free energy, and delta parameter. These values were calculated using the provided code based on the exact composition if available, and an equimolar composition otherwise. The synthesis method corresponds to the categories defined in section 3: 1) High heating and high cooling rate method, 2) Solution-phase (electro)chemical method, 3) Majority component method, 4) Ablation method and 5) Dealloying method.

[illegible]

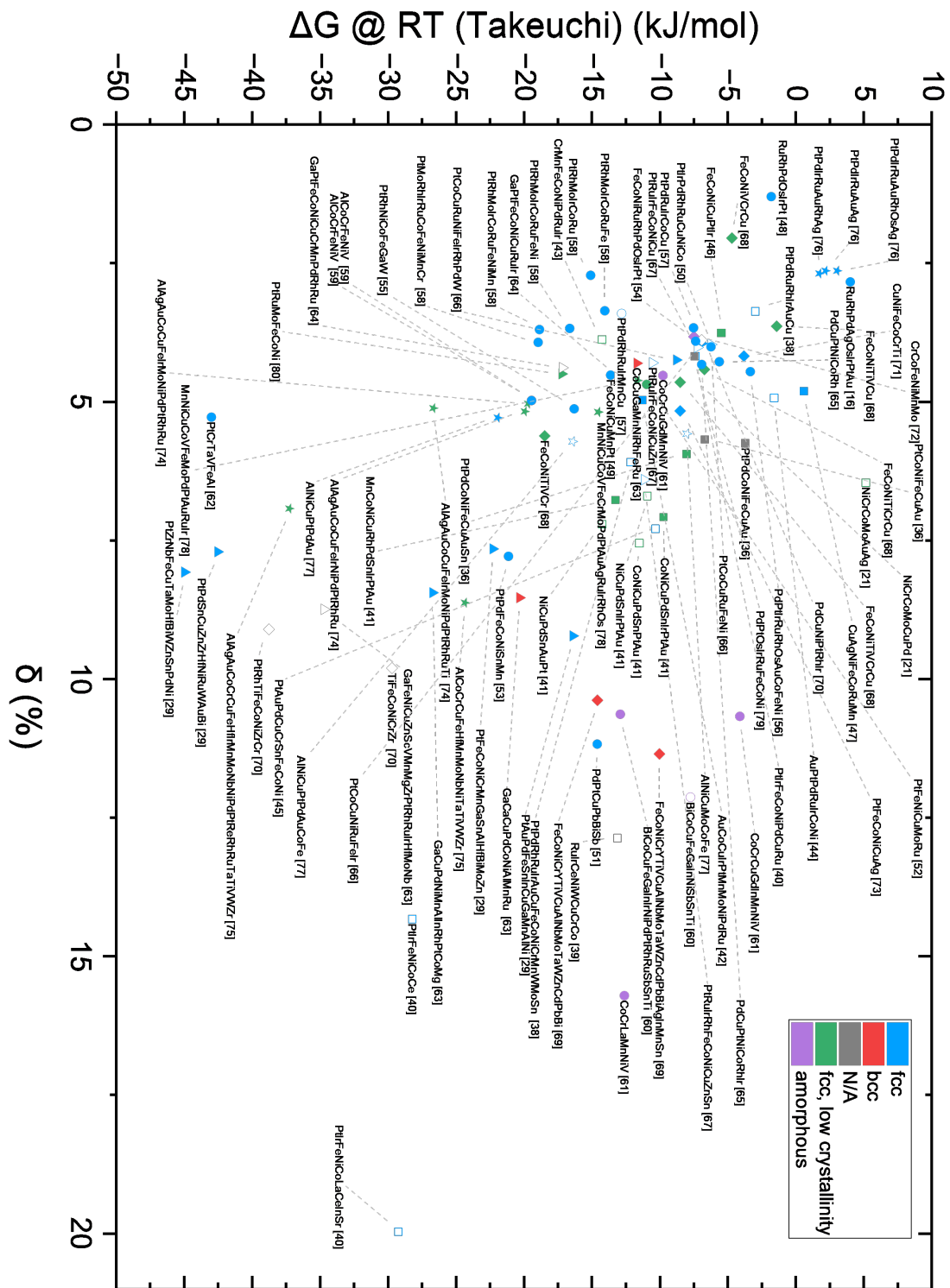


Figure S1: Calculated free energy of mixing at room temperature based on binary enthalpies calculated by the Miedema model by Takeuchi et al. as a function of the delta parameter. The type of crystal system obtained is colour coded. The symbols correspond to the various synthetic methods (squares, high heating and cooling rate methods; circles, liquid-phase (electro)chemical reduction, triangles, majority component method, diamonds; ablation methods; and stars, dealloying). Alloys with known composition are denoted by a full symbol. For unknown alloy compositions, equimolar composition is assumed for calculations, and they are denoted by empty symbols.

