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Effect of crystallography on the calculation energies of equilibrium and enthalpies of formations at first principles calculations (D.F.T)

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Equilibrium energies and enthalpies of formations are calculated based on structural crystallography. Elements and alloys having a large number of atoms are difficult to be compute by density functional theory (DFT): time computation, points of high symmetry.

We have calculated the structural properties, the formation enthalpies and total energies of elements Si, Ni and Au-Re binary compounds (Re = Y, La,Eu) using the first principles calculations based on the density functional theory (DFT) byVasp package.

Comparison of structural properties, formation enthalpies and total energies obtained using firstly the primitive unit cell and secondly the Conventional unit cell of the same phase present a good agreement between the two cases.

The benefits of crystallography allowed the abintio simulator to save computing time; by the exact determination of the atomic positions and symmetry space group of such a material.

Keywords: crystallography, first principles calculation ,enthalpies formation