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### The Search of New Superconducting Materials in Ni – N and Ni –H Systems

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Fe–H and Fe–N systems are well known for their superconducting compounds with transition temperatures up to 50 K. Based on the affinity of iron and nickel atoms we suggested the existence of similar superconductors in Ni–N and Ni–H systems and undertook their theoretical search. The calculations on crystal structure prediction have been performed with evolutionary algorithms (USPEX package) and density functional theory (VASP) package at 100, 200, 300, and 400 GPa. As a result, several new candidates for superconducting materials have been revealed in the Ni-N system. During our investigation, the results on the Ni-H system have been published by Xi and co-authors<sup>1</sup>. The transition temperatures nickel hydrides do not exceed 1 K. In addition to Ni-H and Ni-N systems, we have also performed the search in Fe–H and Fe–N systems. Although no new perspective structures have been found in these systems, we will use them for comparison.

In the system Ni-N, which has not been investigated before, seven new stable structures have been found. The convex-hulls and corresponding sequences of phase transitions for this system are shown in Figure 1. In nitrogen-rich part of the system which is more perspective for superconductors, the new structure NiN<sub>2</sub>-*Pnmm* has been revealed. Found NiN<sub>2</sub>-*Pnmm* is isostructural to FeN<sub>2</sub>-*Pnmm*, which has a transition temperature of 4-8 K<sup>2</sup>. Our calculations of transition temperatures for NiN<sub>2</sub> are in progress, the results will be presented in Conference and in Proceedings.

Despite at ambient conditions nickel shows 2+, 3+, and 4+ valences, while iron only 2+ and 3+, at pressures above 100 GPa, both iron hydrides and iron nitrides are more reached in the number of phases in comparison with their nickel counterparts. However, this can be the consequence of a less thorough search in nickel compounds. In cases, when nickel hydrides or nitrides have the same stoichiometry they are usually isostructural.

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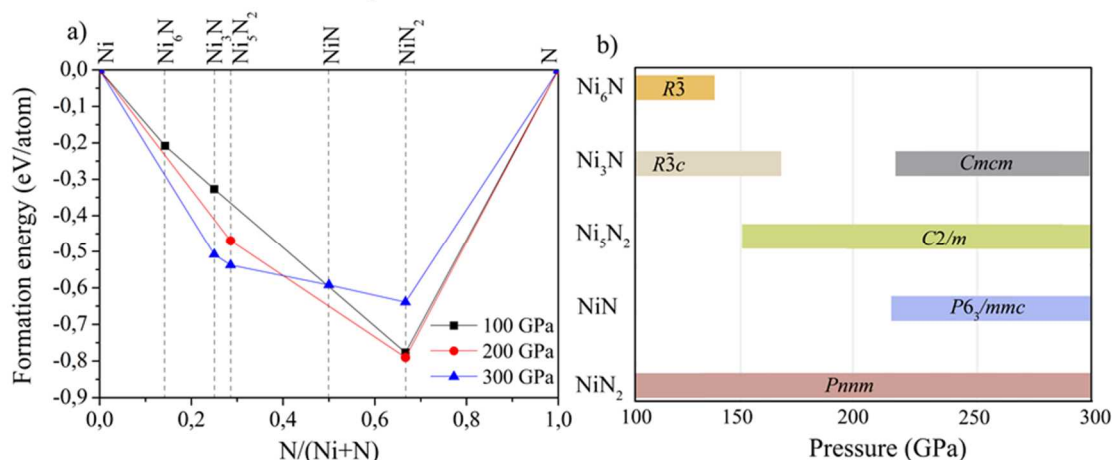


Figure 1. Convex hulls (a) and phase transitions (b) of Ni-N compounds.

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