

## Poster Presentation

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### *Structure variations within certain rare earth-disilicides*

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The dimorphism of the RSi<sub>2</sub> and R<sub>2</sub>TSi<sub>3</sub> compounds is a well known phenomenon (R is an alkaline earth metal, rare earth metal or actinoid, T is a transition metal). They crystallize in structures, which derive from hexagonal AlB<sub>2</sub> or tetragonal ThSi<sub>2</sub> prototypes. Despite their local similarities, both prototypes do not have a common root in the Bärnighausen diagram, which summarizes the symmetry relations between the high symmetrical basic structures and their lower symmetric variations.

We performed an extensive literature research based on more than 400 structure reports of the RSi<sub>2</sub> and R<sub>2</sub>TSi<sub>3</sub> compounds. To gain an overview of the various structure reports within these compounds we summarized composition, lattice parameters *a* and *c*, ratios *c/a*, formula units per unit cell, and structure types in an extensive table. We performed DFT calculations on carefully chosen compounds to evaluate the probability of a successful synthesis. Finally, we discuss peculiarities of symmetry distribution among the RSi<sub>2</sub> and R<sub>2</sub>TSi<sub>3</sub> compounds and several correlations related to structural parameters.

We found that the thermal treatment has a massive effect to the formation of superstructures. Furthermore, there are two different kinds of hexagonal R<sub>2</sub>TSi<sub>3</sub> compounds being ionic or metallic, depending on the R element. Additionally, the main influence to the variation of the Si-T bonds is the electronic interplay between R element and Si lattice rather than the R radii.

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