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**Structural Modifications in Ti-doped NaAlH<sub>4</sub>.** Patrizia Canton, Maximilian Fichtner, Olaf Fuhr, Christoph Frommen, Forschungszentrum Karlsruhe, Inst. of Nanotechnology, P.O.Box 3640, D-76021 Karlsruhe, Germany.

In the search for suitable materials for reversible hydrogen storage, alkali aluminum hydrides such as NaAlH<sub>4</sub> have attracted interest mainly due to the high relative weight of stored hydrogen. NaAlH<sub>4</sub> could be made reversible by doping it with Ti [bogdanovic07]. Furthermore, it is possible to improve the hydrogen exchange kinetics by ball milling in combination with or without additives.

In line with this, there is a considerable interest to the structural properties of pure and doped NaAlH<sub>4</sub>. Moreover, a better understanding of the role of dopants could help in explaining the transformation mechanism of the alanate-dopant composite materials and can provide both higher reversible amounts of hydrogen and improved reaction rates.

Here we report single crystal XRD analysis of purified sodium alanate and powder XRD Rietveld refinement of NaAlH<sub>4</sub>, pure and doped with Ti clusters after 4 absorption/desorption cycles. The aim is to establish the influence of the preparation method on the crystal structure of the pure alanate and to determine the effect of the dopant. A study about the possible substitution of Al or Na cations by Ti and/or the formation of vacancies inside the lattice is reported.