

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Low-Energy Polymeric Phases of Alanates¹ HUAN TRAN, MAXIMILIAN AMSLER, Universität Basel, Switzerland, MIGUEL MARQUES, SILVANA BOTTI, Université de Lyon, France, ALEXANDER WILLAND, STEFAN GOEDECKER, Universität Basel, Switzerland — Low-energy structures of alanates are currently known to be described by patterns of isolated, nearly ideal tetrahedral $[\text{AlH}_4]$ anions and metal cations. We discover that the novel polymeric motif recently proposed for LiAlH_4 plays a dominant role in a series of alanates, including LiAlH_4 , NaAlH_4 , KAlH_4 , $\text{Mg}(\text{AlH}_4)_2$, $\text{Ca}(\text{AlH}_4)_2$ and $\text{Sr}(\text{AlH}_4)_2$. In particular, most of the low-energy structures discovered for the whole series are characterized by networks of corner-sharing $[\text{AlH}_6]$ octahedra, forming wires and/or planes throughout the materials. Finally, for $\text{Mg}(\text{AlH}_4)_2$ and $\text{Sr}(\text{AlH}_4)_2$, we identify two polymeric phases to be lowest in energy at low temperatures.

¹Work supported by Swiss NSF. Computational resources were provided by the Swiss National Supercomputing Center (CSCS) in Lugano.

Huan Tran
Universität Basel, Switzerland

Date submitted: 09 Nov 2012

Electronic form version 1.4