Low-Energy Polymeric Phases of Alanates¹ HUAN TRAN, MAX-IMILIAN 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 [AlH₄] anions and metal cations. We discover that the novel polymeric motif recently proposed for LiAlH₄ plays a dominant role in a series of alanates, including LiAlH₄, NaAlH₄, KAlH₄, Mg(AlH₄)₂, Ca(AlH₄)₂ and Sr(AlH₄)₂. In particular, most of the low-energy structures discovered for the whole series are characterized by networks of corner-sharing [AlH₆] octahedra, forming wires and/or planes throughout the materials. Finally, for Mg(AlH₄)₂ and Sr(AlH₄)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.