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Growth pattern and emergence of bulk-like structures in Aluminum Hydride (AlH_3) nanoclusters GEORGIA MONTONE[1], ANIL KANDALAM, WILLIAM SAWYER, West Chester University, DEPARTMENT OF PHYSICS TEAM — Complex aluminum hydrides, because of their light weight and being hydrogen-rich, have attracted considerable attention as a potential hydrogen storage materials and propellants. In this poster, we will present our computational results exploring the structural evolution and stabilities of neutral and anionic $(AlH_3)_n$ (n = 2-8) nanoclusters. Using density functional theory based calculations of neutral $(AlH_3)_n$ (n=2-8) clusters, we identified a new prototype, based on the unit cell of γ-AlH_3, that forms a template for the growth pattern of higher alanes, n >6. Structures containing hexa-coordinated Al atoms dominate this growth pattern. These findings contradict previous studies which predict ring or polymer-like chain structures for AlH_3 nanoclusters. For anionic $(AlH_3)_n$ clusters, the preference for structures containing hexa-coordinated Al atoms was observed for clusters n >4. The stabilities of these clusters against fragmentation will also be presented and discussed.

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