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Dynamical stability of the cubic metallic phase of AlH3 at ambient pressure DUCK YOUNG KIM, RALPH H. SCHEICHER, Condensed Matter Theory Group, Department of Physics and Materials Science, Uppsala University, Box 530, SE-751 21, Uppsala Sweden, RAJEEV AHUJA, CMT Group, Uppsala; Applied Materials Physics, Dept. of Materials and Engineering, Royal Institute of Technology (KTH), Stockholm — We have characterized the high-pressure cubic phase of AlH_3 using density functional theory to determine mechanical as well as electronic properties and lattice dynamics from the response function method [1]. Metallization in AlH_3 under pressure has been studied, which is of great interest not only from a fundamental physics point of view for the study of phenomena related to metallic hydrogen, but also, because metallic AlH_3 possesses weaker Al-H bonds than other insulating phases [2]. Our phonon calculations show the softening of a particular mode with decreasing pressure, indicating the onset of a dynamical instability that continues to persist at ambient conditions. We find from analyzing the atomic and electronic interactions using theoretical calculations that finite-temperature effects lead to the desired stabilization of metallic AlH_3 at ambient conditions.
[1] PRB **78**, 100102(R) (2008).
[2] APL **92**, 201903 (2008).

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