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Towards a metallic glass transition in α-Al_2O_3: A role of pressure-induced amorphization SANJEEV K. GUPTA, Department of Physics, Michigan Technological University, Houghton, MI-49931, USA, PRAFULLA JHA, Department of Physics, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar-364001, India — Pressure-induced amporphization has been observed experimentally in many electrically insulating materials, including oxides. In none of the cases, the pressure-induced amorphization has been accompanied by metallic conduction. Alumina is one of the most important ceramics of the modern age and has a large band gap of at ambient conditions. In this talk, we will present the results of the study on the behavior of alumina under increasing pressure using first principles plane wave method within the linear response approach. The crystal structure and associated equilibrium lattice constants for α-Al2O3 were obtained by minimizing the calculated total energies as function of a lattice constant. Further, to calculate the entropy and other allied properties, we have used density functional perturbation theory (DFPT). The calculated results show that Al2O3 might turn to metallic glass at pressure achievable in a laboratory.

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