**Abstract**

Aluminium monoflouride is a great candidate for ultracold studies owing to its diagonal Frank-Condon factors and its stability. Our study involves theoretical calculations that pertains to the cooling processes involving AlF. As molecules are more complex than atoms, new methods of cooling mechanisms need to be devised for cooling molecules. This research aims to provide the theoretical background for buffer gas cooling, evaporative cooling and sympathetic cooling methods. We have employed Coupled Cluster (CC) and Multi Reference Configuration Interaction (MRCI) ab initio quantum chemistry methods to calculate the interaction potentials to a high accuracy. The interaction of AlF molecules with each other (tetra atomic system), helium atom (triatomic system) and with Rubidium atoms (triatomic system) have been calculated for ground and excited states of the AlF molecule. High quality potential energy surfaces are reported for all these interactions and the basis set convergence of ab initio methods and effect of relativistic effects were also studied for each of the system. The accuracy and the limitations of ab initio quantum chemistry methodology is also demonstrated. Scattering calculations for the AlF-He collisions were made and provide insight into the experimental prospects of buffer gas cooling of AlF. Data for future scattering calculations are also made available for the AlF-AlF and AlF-Rb interactions which would provide an theoretical basis for the corresponding experiments. One other main result of this study is the full four dimensional interaction potential for AlF-AlF interaction is calculated with significant accuracy.