Ab initio molecular dynamics study of small alkali metal clusters

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In this work, the dynamics of the clusters of the type M3 with M a metal alkaline atom from Li to Cs have been studied. Other heteroatomic mixed clusters like LiNaK and one bigger cluster, Na7, have also been studied. It was found that the dynamics present interesting phenomena like pseudorotations and crossovers which could explain the differences between experimental and theoretical values of some electrical properties, like the electric dipole moment of alkali metal clusters.