

MASTER'S THESIS

Structure and dynamics of doped ionic clusters: a computational study

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**STRUCTURE AND DYNAMICS OF DOPED IONIC
CLUSTERS : A COMPUTATIONAL STUDY**

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A Thesis submitted in partial fulfilment of the requirements for
the degree of Master of Philosophy

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ABSTRACT

This thesis reports numerical computational results obtained for doped NaCl clusters, $\text{ImNa}_n\text{Cl}_{n+2}$ with $n = 1 - 8$. The impurity ion, Im, carries +2 charges but may have various sizes. A new optimization procedure has been designed and used to search for their stable configurations, which differ drastically from the crystal structure in the bulk. From the optimization results, the structures and dynamical response of doped clusters can be studied.

The structural analyses of the calculated optimum configurations are divided into two parts: statics and dynamics. The statics part concerns structural quantities such as the most possible separation, total dipole moment and total interaction energy. Such information tells us how the geometrical and symmetry properties of the clusters are modified by the presence of impurities. The dynamics part of the analysis focuses on vibrational excitations which contribute enormously to the free energy of the clusters at finite temperatures. Vibrational frequencies and density of states are calculated for doped clusters with impurity ions of different sizes. We can study how clustering around a guest ion opens up new channels for the disposal of vibrational energy of the guest. All this information is important for us in understanding the experimental results on melting transitions in clusters, that was found originally in computer simulations.

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