

# A Density Functional Study of $\text{Li}_n\text{Cl}$ ( $n = 1 - 7$ ) Clusters

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The equilibrium geometries, relative stabilities, and electronic properties of  $\text{Li}_n\text{Cl}$  ( $n = 1 - 7$ ) clusters were investigated within the density functional theory (DFT). The lowest energy structures reveal that the impurity chlorine atom prefers the apex position with the coordination number two except the  $\text{Li}_6\text{Cl}$ . From dissociation energy, second-order energy differences, and the energy gaps between highest occupied and lowest unoccupied molecular orbital (HOMO-LUMO),  $\text{Li}_n\text{Cl}$  ( $n = 1, 3, 5$ ) clusters are more stable within the studied cluster range. The binding energy per atom decreases as the cluster size increases, hence the clusters become more reactive when doped with the chlorine atom.

*Key words:* Clusters; Geometrical Configuration; Stability; Density Functional Theory.