

## A theoretical study of alkali metal atomic clusters: From $\text{Li}_n$ to $\text{Cs}_n$ ( $n = 2-8$ )

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A theoretical study of the electronic structure of the first members of the alkali metal atomic clusters series  $\text{Li}_n$  to  $\text{Cs}_n$  ( $n = 2-8$ ) has been done. The geometries of some isomers of the neutral, positive, and negative charged clusters have been determined. Some important properties have also been calculated: atomic binding energies, vertical and adiabatic ionization potentials, vertical and adiabatic electron affinities, static dipole polarizabilities, and energy gaps. Whenever possible they have been compared with experimental values yielding a reasonable agreement which supports some new values as reliable predictions. The data have been discussed in light of the periodic table of elements trends. © 2008 Wiley Periodicals, Inc.