

On the theoretical calculation of the static dipole polarizabilities of Lin, Cun ($n \leq 8$) and LinCum ($n, m \leq 4$)

Fuentealba, Patricio

Padilla-Campos, Luis

Reyes, Orfa

© 2004 IOS Press and the authors. The static dipole polarizabilities of three series of clusters have been calculated and compared. They are the bare lithium clusters, the copper clusters and the mixed lithium-copper clusters. The calculations have been done solving the Kohn-Sham equations with a hybrid exchange-correlation functional. Some discrepancies with the experimental values for lithium clusters have been discussed. It has been found that the dipole polarizabilities of the copper clusters are smaller than the ones of lithium clusters, and the mixed ones follow close the values found for the copper clusters.