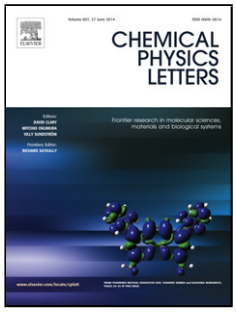

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PII: S0009-2614(15)00920-3
DOI: http://dx.doi.org/doi:10.1016/j.cplett.2015.11.049
Reference: CPLETT 33453

To appear in:

Received date: 30-9-2015
Revised date: 25-11-2015
Accepted date: 27-11-2015

Please cite this article as: H.-S. Hu, Y.-F. Zhao, J.R. Hammond, E.J. Bylaska, E. Apr*gravea*, H.J.J. Dam, J. Li, N. Govind, K. Kowalski, Theoretical studies of the global minima and polarizabilities of small lithium clusters, *Chem. Phys. Lett.* (2015), http://dx.doi.org/10.1016/j.cplett.2015.11.049

Theoretical studies of the global minima and polarizabilities of small lithium clusters

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Abstract: Lithium clusters Li_n (n=1-20) have been investigated with density functional theory (DFT) and coupled-cluster (CC) methods. The global minima are located via an improved basin-hopping algorithm. Simulated polarizabilities are in good agreement with the measured data generally. The simulated polarizabilities for Li_6, Li_{12} and Li_{19} are in reasonable agreement when thermal effects are included. except the Li_3 cluster. A linear correlation for the inverse relationship between the CCSD calculated polarizabilities and ionization potential (IP) has been reported to have the linear coefficient of 0.996, which further strengthens our simulations.

Highlights

for the manuscript with number of "CPLETT-15-1330" and the title of "Theoretical studies of the global minima and polarizabilities of small lithium clusters"