

Abstract Submitted  
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**Stability and Spectroscopic Properties of Singly and Doubly Charged Anions** SWAYAMPBHA BEHERA, PURU

JENA, Virginia Commonwealth University — Considerable interest currently exists in expanding the pool of hetero-atomic negative ions which have electron affinities much higher than that of halogen atoms. These molecules, called superhalogens, usually consist of a metal atom (M) at the core surrounded by halogen atoms (X) and are represented by the formula  $MX_{n+1}$  where n is the maximal valence of the metal atom. We have studied the possibility if pseudohalogens such as CN, which mimic the chemistry of halogen atoms, can be used as building blocks of new superhalogens. Using density functional theory, Moller-Plessett perturbation theory and coupled clusters methods we have studied systematically the structure and spectroscopic properties of  $M(CN)_n$  systems (M=Na, Mg, Al; n=1-3 for Na, 1-4 for Mg, and 1-5 for Al) and compared the results to that of corresponding  $MCl_n$  clusters. We find that there is a significant difference between these two systems. This is because pseudohalogens have a tendency to dimerize and hence, we find that for these clusters the values of adiabatic detachment energy and the electron affinity may not be the same. Also, we have studied the dianions of  $M(CN)_n$  and  $MCl_n$  complexes to determine the critical size required for their stability. We show that CN moieties stabilize a dianion better than halogen atoms do due to the increase in the phase space over which added electrons are delocalized. This could play an important role in interpreting future experimental data on  $M(CN)_n$  complexes.

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