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**Small Metallized Carbon Clusters.** A. PATRICK, P. WILLIAMS, E. BLAISTEN-BAROJAS, School of Computational Sciences, George Mason University, Fairfax, Virginia 22030 — Studies of carbon clusters with 1-4 Ca atoms metallized with Li and Be were performed within the density functional theory approach (DFT). Structures of the ground state and first 3 or 4 excited states where systematically calculated for $C_mLi_n$ and $C_mBe_n$with $n$, $m$=1, 2, 3, and 4. Several of these clusters have ground states of high multiplicity, which make them interesting for magnetic applications. Overall, most stable structures are either linear or planar in the ground state for the smaller clusters, whereas larger clusters acquire 3D structures. Charge transfer in these compounds is notorious, showing no indication of covalent bonding. Calculations were done with DFT the gradient corrections and large basis sets, and compared for several excited states with CASSCF calculations.

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