Density Functional Studies of Magic Metal-$(C_{60})_2$ Clusters EVA
ZUREK, Max Planck Institute for Solid State Research, JOCHEN AUTSCHBACH,
Department of Chemistry, University at Buffalo — Previous experimental studies of
C_{60}-metal clusters revealed that clusters with composition $C_{60}Ba_{32}$ and $(C_{60}K_6)_nK^+$
appeared as magic peaks in the Time-of-Flight mass spectra due to geometric and
electronic stability, respectively. Recent experiments using a new heating technique
have revealed a different set of magic peaks, which cannot be explained by either
one of the aforementioned mechanisms. We present theoretical studies addressing
the stability and bonding of these newly observed magic clusters. Molecular density
functional calculations have been performed to determine the most energetically
stable geometrical configurations for $M_n(C_{60})_2$ clusters, with $M = $ K, Ba and $1 \leq
n \leq 6$. The bonding mechanisms have been analyzed in some detail. The results
indicate that for barium containing clusters, ionic bonding (transfer of the valence
$6s$ electrons to the $C_{60} - \pi^*$ orbitals) and covalent bonding (between the barium $5d$
and $C_{60} - \pi^*$ orbitals) are the dominant mechanisms. Moreover, a metal cluster is
formed between the two fullerenes (Ba-Ba bonding). For the potassium containing
clusters, only ionic bonding was found. Calculations of the Gibbs free energies
indicate that $Ba_3(C_{60})_2$ and $K_4(C_{60})_2$ are the most stable structures, in agreement
with experimental results. The role of the entropy is found to be very important in
determining which clusters are magic.

Eva Zurek
Max Planck Institute for Solid State Research