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Magic Number of a Spherical Ca Cluster on C_{60} SUNGJONG WOO, YOUNG-KYUN KWON, University of Massachusetts Lowell — Since the discovery of fullerenes, there have been a lot of interest in investigating the metal-fullerene clusters. Mass spectrum on the metal(M) covering on a C_{60} complex showed a peak at $M_{32}C_{60}$. This magic number was theoretically explained using the geometry based on the C-Ca binding. However, such theories could not clearly reveal why the peak at $M_{32}C_{60}$, especially for calcium clusters, is so prominent compared to smaller number of metal atoms. Using *ab initio* MD simulations, we have found that for Ca covering with less than 32 atoms, Ca atoms tend to be retracted to a cluster rather than to be bound on each face of C_{60} even though the Ca atoms are deposited symmetrically. Such a cluster does not have specific number of atoms and it is bound to C_{60} through van der Waals interaction. However, once Ca forms a spherical shell with 32 atoms, the structure is quite rigid so that it will not be retracted to a cluster. We have also found that the interaction between an individual Ca atom and each C_{60} face gets loosen so that C_{60} can rotate within Ca_{32} sphere. The phonon spectrum has been obtained by spectral analysis and electronic orbitals of $Ca_{32}C_{60}$ will also be presented.

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