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Gold cluster beyond hollow cage: Double-shell Au_{58} CHUAN-DING DONG, XIN-GAO GONG, Fudan University, Shang Hai, PR China — Gold clusters were found to have planar and hollow cage-like structures due to the strong relativistic effect. By using first principles calculation, we take Au_{58} as an example to demonstrate that gold cluster can show shell structure. Au_{58} reaches its highest stability with an optimal inner core of 10 atoms. Particularly, a double-shell structure with a hollow inner shell shows remarkable robustness. It is significant to consider this shell structure as a descendant of the hollow cage structures found previously, such as tetrahedral Au_{16}, icosahedral Au_{32}, tubular Au_{50} and so on, for this implies a possible evolution from planar, to cage, to shells and finally to the compact structure as the number of atoms in the cluster increasing.

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