Gold cluster beyond hollow cage: Double-shell $\text{Au}_{58}$ 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 $\text{Au}_{58}$ as an example to demonstrate that gold cluster can show shell structure. $\text{Au}_{58}$ 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 $\text{Au}_{16}$, icosahedral $\text{Au}_{32}$, tubular $\text{Au}_{50}$ 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.