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**Geometries and stabilities of Ag-doped $Si_n$ (n =1 - 13) clusters: a first-principles study**[1] FENG-CHUAN CHUANG, YUN-YI HSIEH, CHIH-CHIANG HSU, MARVIN ALBAO, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan — The structures of $AgSi_n$ (n = 1 - 13) clusters are investigated using first-principles calculations. Our studies suggest that $AgSi_n$ clusters with n = 7, and 10 are relatively stable isomers and that these clusters prefer to be exohedral rather than endohedral. Moreover, doping leaves the inner core structure of the clusters largely intact. Additionally, the plot of fragmentation energies as a function of silicon atoms shows that the $AgSi_n$ are favored to dissociate into one Ag atom and $Si_n$ clusters. Alternative pathways exist for n > 7 (except n = 11) in which the Ag-Si cluster dissociate into a stable $Si_7$ and a smaller fragment $AgSi_{n-7}$. The $AgSi_{11}$ cluster dissociates into a stable $Si_{10}$ and a small fragment AgSi. Lastly, our analysis indicate that doping of Ag atom significantly decreases the gaps between the highest occupied molecular orbital and the lowest unoccupied molecular orbital for n > 7. Reference: J. Chem. Phys. 127, 144313 (2007).

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