The influence of palladium doping on the geometry and the stability of small cationic gold clusters

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Small gold clusters are unique objects with fascinating features, such as the surprisingly larger sizes up to which the clusters are two-dimensional [1]. Their properties are strongly dependent on the precise number of atoms in the cluster, as reflected in most electronic-structure related features, including optical responses [2], size-to-size stabilities [3] and reactivities [4]. Doping can significantly modify the properties of the clusters, allowing a high degree of tunability [5]. From a fundamental point of view, palladium is a very interesting dopant atom, since its ground-state electronic configuration has a closed 4d shell and no valence s electrons ([Kr]4d^{10}), in contrast to gold, with a closed 5d shell and one 6s valence electron ([Xe]4f^{14}5d^{10}6s^{1}). In this work, we analyse in detail how doping Au_n^+ ($n \leq 11$) with Pd modifies their geometry and electronic structure, and how this determines the stability of the clusters. Structural information is obtained by far-infrared multiphoton dissociation spectroscopy in combination with density functional theory calculations, whereas photofragmentation experiments are used to investigate the size dependent stabilities [6].

References

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