Iron Doped Gold Cluster Nanomagnets: *Ab Initio* Determination of Barriers for Demagnetization

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Magnetic properties of small- and nano-sized iron doped gold clusters are calculated at the level of second order multireference perturbation theory. We first assess the methodology for small Au_6Fe and Au_7Fe clusters, which are representative of even and odd electron count systems. We find that larger active spaces are needed for the odd electron count system, Au_7Fe, which exhibits isotropic magnetization behaviour. On the other hand, the even electron count system, Au_6Fe, exhibits strong axial magnetic anisotropy. We then apply this methodology to the tetrahedral and truncated pyramidal nano-sized $Au_{19}Fe$ (with S=3/2) and $Au_{18}Fe$ (with S=2) clusters. We find that face substitutions result in the most stable structures, followed by edge and corner substitutions. However, for $Au_{18}Fe$, corner substitution results in strong magnetic anisotropy and a large barrier for demagnetization while face substitution does not. Thus, although corner and face substituted $Au_{18}Fe$ have the same spin, only corner substituted $Au_{18}Fe$ can act as a single nanoparticle magnet.

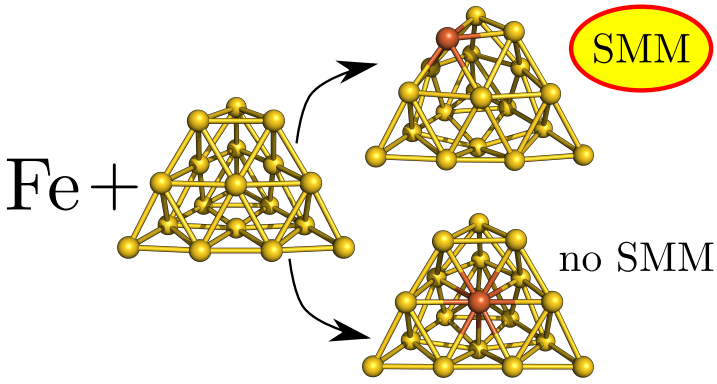

Figure 1: Single molecule magnet properties depend on the substitution scheme.

References

1. C. Ehlert and I. P. Hamilton, *Nanoscale Adv.* **1** (2019), 1553.