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$_6$Fe and Au$_7$Fe 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$_7$Fe, which exhibits isotropic magnetization behaviour. On the other hand, the even electron count system, Au$_6$Fe, 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