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\(_6\)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
1. C. Ehlert and I. P. Hamilton, *Nanoscale Adv.* 1 (2019), 1553.