Aluminium/Gold Clusters as building blocks for new metastable polymorphs.

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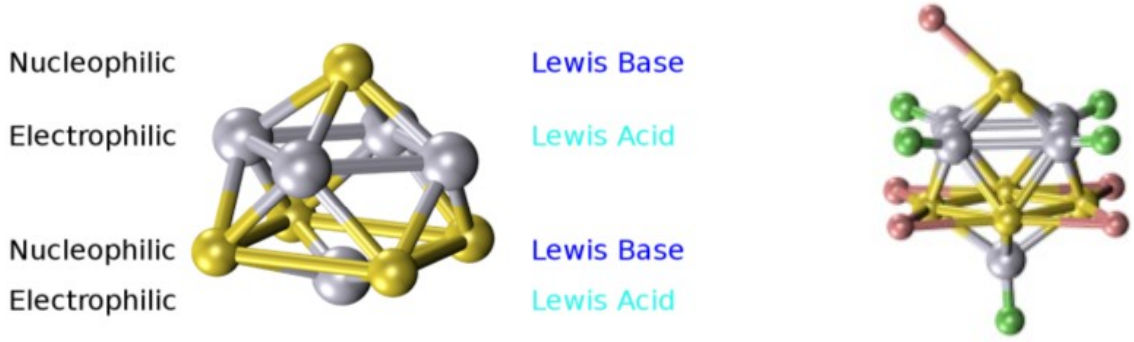
The structural and optical properties of both, the naked and passivated bimetallic Al_5Au_5 nanocluster have been analyzed based on data obtained from ab initio density functional theory and quantum molecular dynamics simulations. It has been found that the Al_5Au_5 nanocluster posses a hollow shaped minimum energy structure with segregated Al and Au layered domains, the former representing the electrophilic domain and the latter the nucleophilic domain (see below, in the left). In particular, it has been shown that alkali metal cations attach in the nucleophilic domain and hop from one Au site to the next one in the picoseconds time scale, while anions bound tightly to the Al atoms of the electrophilic domain (see below, in the right). Simulating annealing studies are very suggestive of the proneness of the nanocluster towards coalescence into large cluster units, when the cluster is left unprotected by appropriate ligands. Further passivation studies with NaF salt suggest, nonetheless, the possibility of the isolation of the Al_5Au_5 cluster in molten salts or ionic liquids[1].



References

1. R. Grande-Aztatzi, E. Formoso, J. M. Mercero, J. M. Matxain, S. J. Grabowski, J. M. Ugalde, *J. Chem. Phys.*, **144**, 114302 (2016).