Nanocluster collisions as a way to understand the role of d-shell polarization

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Collision processes between single gold and rhodium atoms and gold and rhodium nanoclusters, respectively, are used to study the interplay between the large elastic energies and the much smaller magnetic interactions. The latter, in spite of their small magnitude, often settle the configuration of crystals, clusters, and molecules. We implement ab initio molecular dynamics (DFT-MD) calculations to investigate the subtle balance between these two forces. The targets we consider are minimum energy 13 (12) atom gold (rhodium) clusters. Results for gold and rhodium are compared emphasizing the relevance of d-shell polarization. The use of these collision processes to generate putative nanocluster minimum energy configurations will be presented and illustrated with successful examples.