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Non-uniquely defined ground states of a neutral and anionic gold cluster and methods for generating stationary point databases BASTIAN SCHAEFER, University of Basel, RHITANKAR PAL, Yale University, MAXIMILIAN AMSLER, ALI SADEGHI, University of Basel, XIAO CHENG ZENG, University of Nebraska-Lincoln, LAI-SHENG WANG, Brown University, VOLKER BLUM, Duke University, STEFAN GOEDECKER, University of Basel, GOEDECKER GROUP TEAM, ZENG GROUP TEAM, WANG GROUP TEAM, BLUM GROUP TEAM — Using the Minima Hopping structure prediction method at the density functional level, we found new low energy minima for mid-sized neutral and singly charged anionic gold clusters. We demonstrate that the local- density and a generalized gradient approximation of the exchange-correlation functional predict different structural motifs. For both the anionic and the neutral system there exist a vast number of structurally different isomers within a small energy window above the putative global minima. Consequently, no uniquely defined ground states are expected to exist for these systems at finite temperatures. For the anionic system we present a disconnectivity graph that has been build completely at the density functional level. The transition states used to build this disconnectivity graph are complete enough in order to predict that the anionic system could have a fluxional shell, which may implicate catalytic activity for this cluster. We also discuss methods to generate stationary point databases required for the generation of disconnectivity graphs.

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