Exploring the Structure-Dependent Stability of Thiolated Metal Nanoparticles

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"Magic numbers" in the stability of $M_n(SR)_m$ nanoparticles and their corresponding atomically-precise structures have recently been identified with advancements in experimental synthesis and characterization techniques.[1,2] Traditionally, this experimentally observed magic stability has been explained by electron-counting methods such as the "superatom model".[3] However, this model has not held in rationalizing the stability of several recently-identified nanoparticle structures, such as the $Au_{20}SR_{16}$ and the $Au_{36}SR_{24}$.[4] Herein, we introduce a theory developed utilizing density functional theory calculations relating the stability of the overall thiolated-metal nanoparticles to structure-dependent descriptors. Using the identified descriptors we rationalize the stability of various monometallic atomically-precise nanoparticles both for charged and neutral systems. Our findings aid in accelerating the discovery of atomically precise, stable metal nanoparticles and suggest a new way of rationalizing thermodynamic stability in nanoscale systems.

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