Abstract Submitted
for the OSF16 Meeting of
The American Physical Society

Relationship between HOMO-LUMO gap and stability of noble metal molecular nanoparticles (MNPs) in gas and condensed phases AYDAR ATNAGULOV, The University of Toledo, SAMEERA WICKRAMASINGHE, Case Western Reserve University, TERRY BIGIONI, The University of Toledo, BIGIONI GROUP TEAM — The energy difference between the highest occupied and lowest unoccupied molecular orbitals, the HOMO-LUMO gap, is often used to rationalize the stability of noble gas atoms, transition metal complexes, and gas phase metal clusters. In the latter case, electrons delocalized across the metal atoms occupy orbitals that are analogous to atomic orbitals such that the cluster may be treated as a "superatom". In the gas phase, it has been shown that bare metal clusters with closed electronic shells exhibit higher stability compared to those with incomplete shells. In the condensed phase, the HOMO-LUMO gap has also been adopted to characterize the expected stability of ligand-protected clusters, but the extent to which this is correct remains untested. Here, we address the relationship between HOMO-LUMO gap and gas and condensed phase stabilities using a binary system of M3Ag17(TBBT)12 and M4Ag44(TBBT)30, where TBBT is 4-tert-butylbenzenethiol and M is an alkali metal. Gas phase stabilities of these nanoparticles were evaluated by measuring their fragmentation using mass spectrometry. Condensed phase stabilities were evaluated by analyzing the composition of solutions at different time points. We found that the HOMO-LUMO gap correlated with gas phase stability, but the cluster with the smaller HOMO-LUMO gap was more stable in solution. This implies that the notion of an energy gap fails to predict stability in the condensed phase.

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Date submitted: 11 Sep 2016 Electronic form version 1.4