Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Site-specific polarizabilities as descriptors of metallic behavior in atomic clusters[1] KOBLAR JACKSON, Physics Department and Science of Advanced Materials Ph.D. Program, Central Michigan University, JULIUS JELLINEK, Chemical Sciences and Engineering Division, Argonne National Laboratory — The electric dipole polarizability of a cluster is a measure of its response to an applied electric field. The site specific polarizability method decomposes the total cluster polarizability into contributions from individual atoms and also allows it to be partitioned into charge transfer and electric dipole contributions. By systematically examining the trends in these quantities for several types of metal atom clusters over a wide range of cluster sizes, we find common characteristics that uniquely link the behavior of the clusters to that of the corresponding bulk metals for clusters as small as 10 atoms. We discuss these trends and compare and contrast them with results for non-metal clusters.

[1]This work was supported by the Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences, U.S. Department of Energy under Grant SC0001330 (KAJ) and Contract No. DE-AC02-06CH11357 (JJ).

Koblar Jackson
Central Michigan University

Date submitted: 20 Nov 2016 Electronic form version 1.4