

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

The evolution of dielectric properties of sodium, silicon and argon clusters¹ KOBLAR JACKSON, Department of Physics, Central Michigan University, Mt. Pleasant, MI 48859, MINGLI YANG, Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, China, LI MA, Department of Physics, Northwest University, Xi'an 710069, China, JULIUS JELLINEK, Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL 60439, USA — We used a computational scheme based on site-specific polarizabilities to study the evolution of the dielectric properties of sodium, silicon and argon clusters. In this approach, the total cluster polarizability is decomposed into local dipole (LD) and charge-transfer (CT) parts. The local dipole part measures the redistribution of charge within an atomic volume, while the CT part describes the movement of charge between volumes. We find distinct differences in the relative contributions of the LD and CT components to the total polarizability as a function of cluster size for the different cluster types and relate this to the development of metallic behavior. The method also directly probes the extent of electrostatic screening of the cluster interior to an applied electric field.

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

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Date submitted: 21 Nov 2011

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