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Atomistic Dipole Moments and Polarizabilities of Na_N Clusters, N= 2-30, 38, and 55.[1] KOBLAR JACKSON, LI MA, Central Michigan University, Mount Pleasant, MI 48859, MINGLI YANG, Institute for Nanobiomedical Technology and Membrane Biology, West-China Medical School/West-China Hospital, Sichuan University, Chengdu, China, JULIUS JELLINEK, Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne IL 60439, USA — The response of Na_N clusters, N = 2 - 30, 38, and 55 to a static external electric field is studied using a new method that decomposes the total cluster dipole moment and polarizability into contributions from non-overlapping atomic volumes (Jackson et al., J. Chem. Phys. **129**, 144309 (2008)). The atomic dipole moments and polarizabilities are in turn partitioned into local dipole and charge-transfer components, corresponding to dielectric and metallic responses, respectively. Analysis of the atomic polarizabilities indicates a strong dependence on the location of the atoms within the clusters and shows directly the effect of electrostatic screening in the clusters. We show that the relative importance of the charge-transfer component of the cluster polarizability increases with cluster size and approaches the bulk-limit on a per-atom basis for clusters as small as 20 atoms. The charge-transfer component is shown to be responsible for the structure/shape driven variations, and for shape-related anisotropies, in the cluster polarizabilities.

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