Abstract Submitted
for the TSS14 Meeting of
The American Physical Society

Dielectric properties of endohedral fullerenes SHUSIL BHUSAL, RAJENDRA ZOPE, TUNNA BARUAH, Univ of Texas, El Paso, KOBLAR JACKSON, Central Michigan University, Mount Pleasant — We investigate the response of the applied static electric field to a series of endoherdal fullerenes using density functional theory. Using an approach to obtain the site-specific polarizabilities implemented in our massively parallel NRLMOL code, we examine the screening of the applied electric field by the pi-electrons on the fullerene cage. In the site specific polarizability scheme, 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. Our results show distinct differences in the relative contributions of the LD and CT components to the total polarizability in endohedral fullerenes and that fullerene cages behave, to a significant extent, as Faraday cages.

Shusil Bhusal
Univ of Texas, El Paso

Date submitted: 28 Feb 2014 Electronic form version 1.4