Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Fully ab-initio study of the optical response of charged rare gas clusters[1] FERNANDO NOGUEIRA, Center for Computational Physics and Physics Department, University of Coimbra, Portugal, MICAEL OLIVEIRA, Center for Computational Physics, University of Coimbra, Portugal and European Theoretical Spectroscopy Facility, MIGUEL MARQUES, LPMCN, Université Lyon I, Lyon, France and European Theoretical Spectroscopy Facility — Charged rare-gas clusters are markedly different from their neutral, van der Waals bonded counterparts. The removal of an electron from a strongly antibonding orbital causes the bonding to become much stronger and shifts the optical absorption to the visible region. We report a fully ab-initio determination of the geometry, electronic structure, and optical response of small singly charged Ne, Ar, Kr and Xe clusters. All calculations were performed using a pseudopotential based real space implementation of Time-Dependent Density-Functional Theory. We find that GGA leads, in general, to much better results than LDA, even though it predicts some absorption peaks at slightly higher energies than those found experimentally. The lighter elements show a single absorption peak but in the heavier elements spin-orbit interaction induces a splitting of the absorption peak, in good agreement with experiment.

[1]This work was supported by Fundação para a Ciência e Tecnologia through grants #POCI/FIS/58309/2004 and #SFRH/BD/12712/2003.

Fernando Nogueira
Center for Computational Physics and Physics Department,
University of Coimbra, Portugal

Date submitted: 27 Dec 2007 Electronic form version 1.4