Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Adaptive Clustering of Adatoms Around Ionic Dopants in He Droplets: Quantum Calculations FRANCESCO A. GIANTURCO, Dept. of Chemistry, University of Rome "La Sapienza" — The structuring and collocation of individual He atoms as quantum objects around simple atomic and molecular impurities has been the subject of a great number of studies, both experimentally and from the theoretical viewpoint [1,2] since the advent of droplets experiments, where such nanoscopic containers have been exploited to provide a sort of nanocryostat for the analysis of the dopant's spectroscopic behavior [3]. We have carried out computations of potential fields within small clusters which contain a variety of ionic dopants using post-Hartree-Fock, ab initio methods and have further endeavoured to extract from them the corresponding classical and quantum structuring of such impurities within clusters of variable size. For the latter enquiry we have employed both classical optimization methods and Quantum Diffusion Monte Carlo analysis. Results for both atomic (Li^+) and molecular (LiH^+, OH^+, OH^-) ionic dopants will be presented at the meeting.

[1] J.P. Toennies and A.F. Vilesov, *Angewandte Chemie* **43**, 2622 (2004).
[2] e.g. see: F. Paesani, A. Viel, F.A. Gianturco and K. Whaley, *Phys. Rev. Lett.* **90**, 073401 (2003).
[3] J.P. Toennies and A.F. Vilesov, {\it Ann. Rev. Phys. Chem.} {\bf 49}, 1 (1998).

Francesco A. Gianturco
Dept. of Chemistry, University of Rome "La Sapienza"

Date submitted: 01 Dec 2005 Electronic form version 1.4