Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Structural and Electronic Properties of (HAlO)$_n$ Clusters YI DONG, MICHAEL SPRINGBORG, University of Saarland, Saarbruecken, Germany — HAlO is a nanostructured material that can be used as a substrate for organized structures of organic molecules. However, except for the fact that HAlO is stoichiometric, very little is known about its structural and electronic properties. Using two different unbiased methods for structure optimization (our own *Aufbau* method as well as Genetic Algorithms) together with a parameterized density-functional method in calculating the total energy and the electronic properties for a given structure, we have optimized the structure of (HAlO)$_n$ clusters with n up to 26. We shall briefly outline our theoretical approach and subsequently present the results for isolated (HAlO)$_n$ clusters together with those for interacting (HAlO)$_n$ clusters and for layers of HAlO.

Michael Springborg

Date submitted: 22 Nov 2004   Electronic form version 1.4