Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Multiple Isomers in the Photoelectron Spectra of NbC_n clusters

IVAN IORDANOV, JORGE SOFO, Department of Physics, Penn State — We calculate the photoelectron spectrum of small NbC_n clusters ($2<n<7$), to identify the atomic structure that best matches experimental photoelectron spectra. We use Density Functional Theory calculations to find all stable isomers. In order to obtain more accurate spectra, we use the Symmetry Adapted Cluster Configuration Interaction method for the smaller clusters where the highly correlated niobium d-orbitals dominate the electronic structure. The most stable isomer configurations are linear and cyclic structures, with the cyclic being the ground state for all but NbC_6. To fully explain all experimental observations we are required to use the combined spectra of both ring and linear structures. This means that both structures must be present in the cluster beam, even in cases where the higher energy isomer is up to 0.5 eV higher than the ground state. This surprising result is confirmed by both DFT and Configuration Interaction.

Jorge Sofo
Penn State

Date submitted: 18 Nov 2008 Electronic form version 1.4