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**Geometric and electronic structure of mixed metal-semiconductor clusters from global optimization.-**

FRANK HAGELBERG, JIANHUA WU, Jackson State University — In addition to pure metal and semiconductor clusters, hybrid species that contain both types of constituents occur at the metal-semiconductor interface. Thus, clusters of the form  $\text{Cu}(x)\text{Si}(y)$  were detected by mass spectrometry [1]. In this contribution, the geometric and energetic features of  $\text{Me}(m)\text{Si}(7-m)$  ( $\text{Me}=\text{Cu}$  and  $\text{Li}$ ) clusters are discussed. The choice of these systems is motivated by the structural similarity of the pure  $\text{Si}(7)$ ,  $\text{Li}(7)$ , and  $\text{Cu}(7)$  systems which all stabilize in  $D(5h)$  symmetry. On the other hand,  $\text{Li}$  and  $\text{Cu}$ , representing the alkali group (IA) and the noble metal group (IB) of the periodic system, are expected to display strongly differing behavior when integrated into a  $\text{Si}(n)$  cluster, resulting in different ground state geometries for the cases  $\text{Me} = \text{Li}$  and  $\text{Me} = \text{Cu}$ . Addressing this problem by means of geometry optimization requires, in view of the large number of possible atomic permutations for  $\text{Me}(m)\text{Si}(7-m)$  with  $0 < m < 7$ , the use of a global search algorithm. Equilibrium geometries are obtained by simulated annealing within the Nose' thermostat frame. It is observed that  $\text{Cu}(m)\text{Si}(7-m)$  clusters with  $m < 6$  tend towards ground state geometries derived from the  $D(5h)$  prototype. For  $\text{Li}(m)\text{Si}(7-m)$ , the  $\text{Li}(m)$  subsystem is found to adsorb on the framework of the  $\text{Si}(7-m)$  dianion. [1] J.J. Scherer, J.B. Pau, C.P. Collier, A. O'Keefe, and R.J. Saykally, J. Chem. Phys. 103, 9187 (1995).

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