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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 Cu(x)Si(y) were detected by mass spectrometry [1]. In this contribution, the geometric and energetic features of Me(m)Si(7-m) (Me=Cu and Li) clusters are discussed. The choice of these systems is motivated by the structural similarity of the pure Si(7), Li(7), and Cu(7) systems which all stabilize in D(5h) symmetry. On the other hand, Li and 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 Si(n) cluster, resulting in different ground state geometries for the cases Me = Li and Me = Cu. Addressing this problem by means of geometry optimization requires, in view of the large number of possible atomic permutations for Me(m)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 Cu(m)Si(7-m) clusters with $m < 6$ tend towards ground state geometries derived from the D(5h) prototype. For Li(m)Si(7-m), the Li(m) subsystem is found to adsorb on the framework of the 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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