Structural and Electronic Properties of $\text{(HAIO)}_n$ Clusters

YI DONG, MICHAEL SPRINGBORG, University of Saarland, Saarbruecken, Germany — HAIO is a nanostructured material that can be used as a substrate for organized structures of organic molecules. However, except for the fact that HAIO 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 $\text{(HAIO)}_n$ clusters with $n$ up to 26. We shall briefly outline our theoretical approach and subsequently present the results for isolated $\text{(HAIO)}_n$ clusters together with those for interacting $\text{(HAIO)}_n$ clusters and for layers of HAIO.