Abstract Submitted
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A study of Au adsorption on yttrium disilicide nanowires on Si (001) substrate from first principles[1] WENJIE OUYANG, University of California, Irvine, ANIKETA SHINDE, JUEXIAN CAO, RUQIAN WU — Core-shell nanoclusters with Au coating layer on uniformly dispersed rear-earth disilicide nanowires are very promising for various applications such as nanocatalysis. Using the first principles approach, we studied the structure and electronic properties of a single Au atatom on yttrium disilicide nanowires on the Si(100) substrate. A series of possible adsorption sites were explored and we found that the "hollow" site on the YSi2 nanowire is the most preferential one, where the Au adatom binds to two Si atoms and an Y atom underneath. The most stable site for Au on Si(001) is the "cave" site, but the binding energy is 0.11 eV higher than that on the wire. This indicates that the Au atoms tend to aggregate toward nanowires, which leads to growth of core-shell metallic structures. Electrons deplete from Au adatom and accumulated in regions between Au and Si. The chemical activity of Au/YSi2 will be discussed in light of charge density, density of states and adsorption energy of CO molecules.

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