

# First-principles calculations of complex metallic alloy surfaces

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We studied the adsorption of pentacene on the 2-fold surface of an icosahedral Ag-In-Yb quasicrystal [1](QC). An STM experiment reported that pentacene molecules adsorbed in a quasiperiodic manner on this surface[2].

The QC surface has approximated by a disk-shaped atomic cluster with a radius of 2.2 nm (Fig. 1). Atomic positions of the QC surface has extracted from the structural data of an X-ray diffraction experiment for the isostructural  $\text{Cd}_{5.7}\text{Yb}$  quasicrystal[3], where Ag and In atoms occupy the Cd sites in the Ag-In-Yb QC. In the calculations, the molecular axis of pentacene is constrained to be parallel to the surface, and all atomic positions, including the substrate atoms, are fixed. Calculations are carried out with the VASP code mainly on the system-B as bulk jobs using 72 nodes.

First, we carefully checked the cluster thickness dependence of the adsorption energy. And we confirmed that the thin film composed only of the top layer atoms well describes the interactions with pentacene. Thus, we describe the results below using the thin film as the substrate.

The adsorption energy of pentacene shows strong orientational dependence on the molecular axis of pentacene. Figures 2(a) and (b) show the adsorption energies of pentacene with its molecular axis aligned to two different 2-fold axes, 2f-90° and 2f-180°, which are parallel to the surface and perpendicular to each other. It is clearly shown that pentacene favors one of them (2f-90° direction shown in

Fig. 2(a)). Comparably stable orientational configurations are found when the molecular axis is aligned to two 5-fold axes on the surface. Obtained orientational dependence of the adsorption energy well explains the result of statistical analysis from an STM experiment[2].

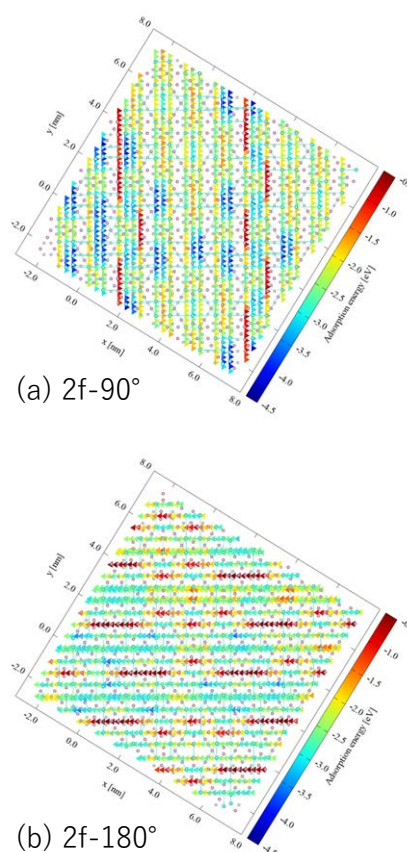


Figure 1: Adsorption energy of pentacene with the molecular axis parallel to the 2-fold (a) 90° and (b) 180° directions.

We also studied the adsorption of oxygen atoms on the (111) surface of the PdZn inter-

metallic compound. We used the VASP code with a slab model consisting of six atomic layers. Using a 2x2 unit cell containing eight atoms in the top layer, we investigated the adsorption structures for various oxygen coverages between 0.125 - 1.0 monolayer (ML). Calculations were mainly carried out on the system-C as flat MPI jobs with 4-9 nodes. At high oxygen coverages, we found that Zn atoms form a Zn-O layer with a hexagonal ring reminiscent of the Wurtzite ZnO. PdZn is known as a candidate catalyst for the methanol steam reforming (MSR) because of its higher thermal stability than the traditional Cu-based catalyst. It has been reported that a ZnO patch is formed on the PdZn catalyst during the MSR reaction, and considered that the high CO<sub>2</sub> selectivity of PdZn in MSR is due to the formation of the ZnO patch[4]. However, there is still no report of the first-principles calculations about the formation of the Zn-O layer.

## References

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