A first principles investigation of a benzene-vanadium multiple-decked sandwich chain on a gold surface

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Molecular magnets have the advantage of being smaller in size compared to bulk magnetic materials. This makes them promising candidates for magnetic storage and spintronics and for developing technologies that could enable computers to have ultra-big storage capabilities [1]. A new type of molecular magnet known as multiple-decked sandwich cluster has been attracting attention recently. Many of these multiple-decked sandwich clusters are synthesized in the gas phase by laser vaporization. Of special interest is the vanadium- benzene cluster because of its stability [2].

In our previous studies, we have investigated electric and magnetic properties of benzene-transition metal multiple-decked sandwich cluster and chain [3-5] using first principles calculations based on density functional theory. In this presentation, we investigate the formation and magnetic properties of benzene-vanadium multiple-decked sandwich chain (BVMSC) on Au(111) surface where the surface consists of a layer of gold atoms. Experimentally, Nakajima's group has succeeded in adsorbing $V(C_6H_6)_2$ cluster on this surface [6]. We show that the BVMSC forms on the surface and find that this system has no magnetic moment for which the two succeeding vanadium atoms are antiferromagnetically arranged. We also suggest a superexchange mechanism for this antiferromagnetic behavior.

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