

Abstract Submitted
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Density-functional study of adsorption of isocyanides on the gold (111) surface.¹ YULIA GILMAN, PHILIP B. ALLEN, Department of Physics and Astronomy, SUNY Stony Brook — Density functional theory (DFT) is used to study how the isocyanides HNC and CH₃NC attach to the gold (111) surface. Slab calculations are performed for monolayers with 1 molecule per 3 gold atoms coverage. For both molecules a weak binding of about 0.2 eV is found at the top site. No binding is found at other sites.

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