Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Evidence of graphene like Sn-Sheet on Au(111) substrate: Electronic structure and transport properties from first principles calculations

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Supporting Information

Table-S1: Comparison of binding energy relevant gas phase dimers.

(Expt. Values : 2002 CRC Handbook of Chemistry and Physics, 83rd ed.; (CRC Press: Boca Raton, FL))

	Binding Energy, eV		Bond Lengh, A	
	This work	Exp	This work	Exp
Sn-Sn	2.36	2.04	2.80	2.76
Au-Sn	2.94	2.49	2.51	
Au-Au	2.38	2.31	2.52	2.47

Table-S2: Comparison of bader charge on Sn-Au systems.

	bader Charge on Sn atom
Sn-Au dimer	+1.33
Sn@Au(111)	+2.06
Sn2@Au(111)	+1.82 Per Sn atom

Table-S3: Comparison of DOS spectrum for the adsorption of Sn/Sn_2 on Au(111) surfaces.

Species	Binding energy(eV) (gas phase)	Adsorption energy(eV)
Sn atom	-	-3.35[&]
2 Sn atoms adsorbed separately as atomic tin placed far apart (3-4 Å away; two neighboring fcc site) on the Au (111)surface	-	-4.33[$]
Sn_2 dimer (The two Sn atom adsorbed on surface with a Sn-Sn bond)	-2.36 eV	-4.41[$]

[&]Adsorption energy for single Sn atom adsorption on Palladium surface ΔE = E [Sn/Au(111)] – E[Au(111)] - E(Sn atom)

[$]Adsorption energy for Sn_2 adsorption on Palladium surface ΔE = E[Sn_2/Au(111)] – E[Au(111)] – E[Sn_2 dimer)]

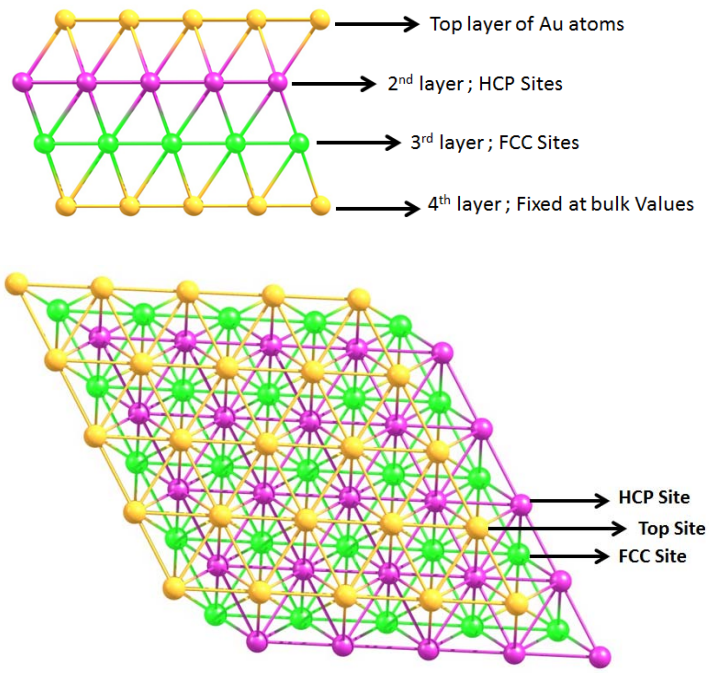


Figure S1: Top, HCP and FCC sites on the Au (111) surface

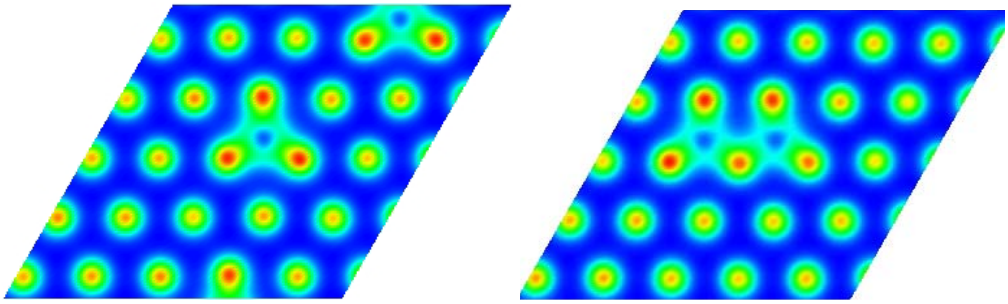


Figure –S2: The iso-surface density of Sn_2@Au111 in (a) far apart (b) bonded case. In both case charge has been transferred to nearby gold atoms.

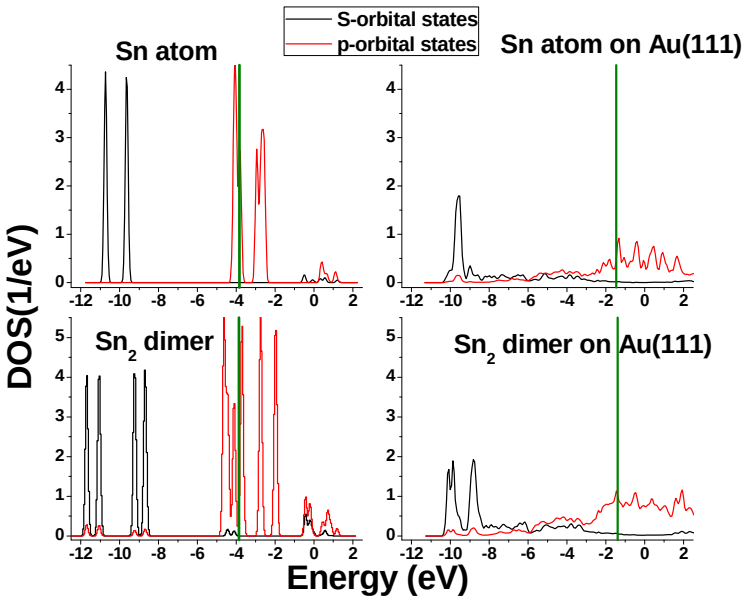


Figure –S3: The DOS of Sn atom and Sn_2 in (a) gas phase (b) deposited on gold surface.

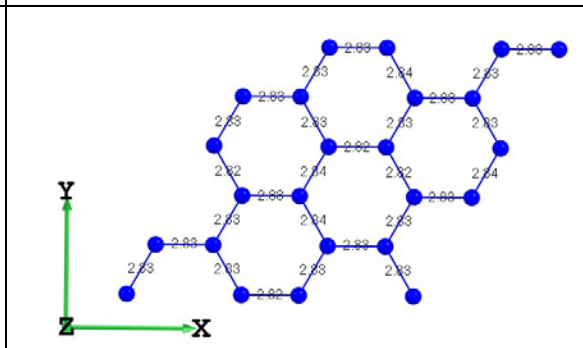
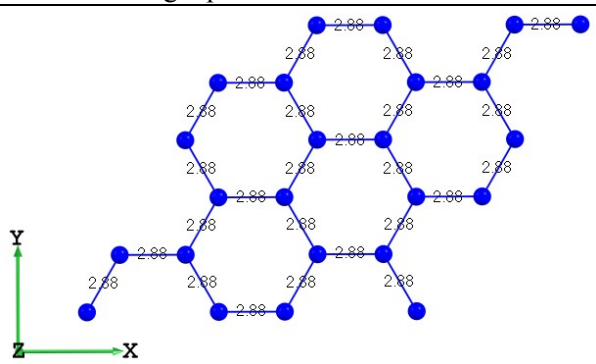
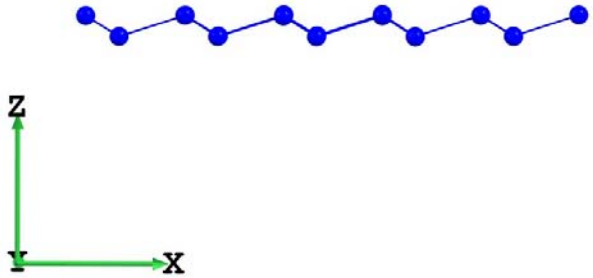
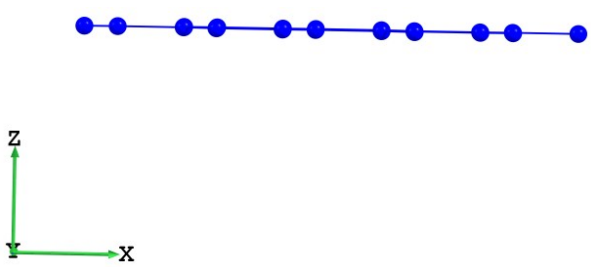
	Free Sn sheet	single point calculation sheet
		
		
	Sn-Sn bond: 2.83 Å	**Sn-Sn bond: 2.88 Å**
Energy	**ΔE = 0.00 eV**	**ΔE = 0.09 eV**
BE	**BE = 2.54 eV/atom**	**BE = 2.35 eV/atom**

Figure S4: Sn Sheet in free state (buckled) compare with the planar Sn sheet obtained by single point calculation on isolated tin sheet detached from Sn@Au(111) configuration.

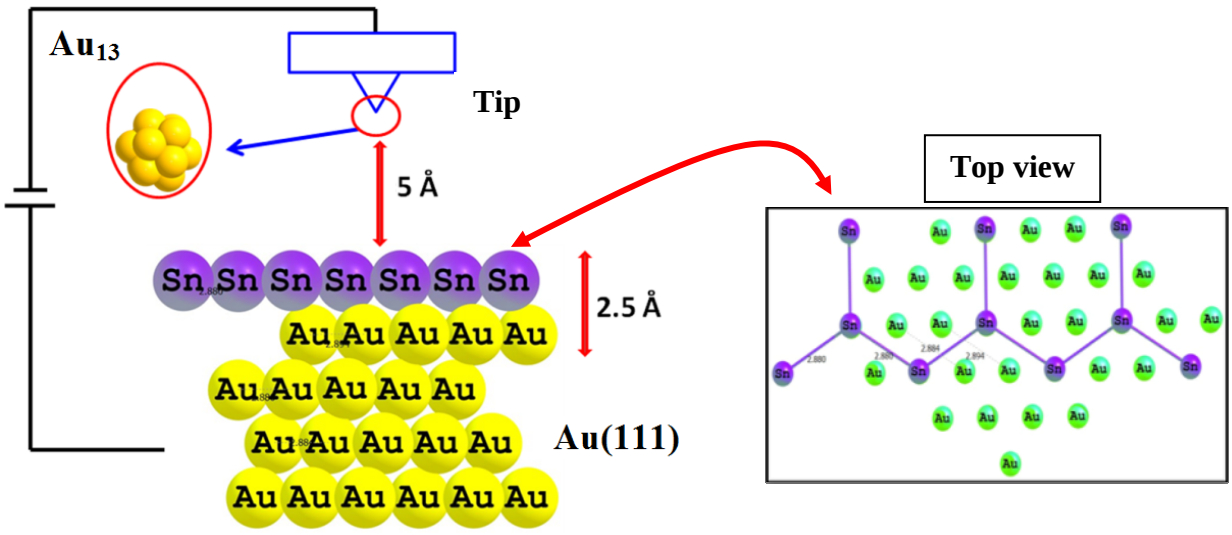


Figure S5. (Color online) (left) A schematic illustration of the STM-like setup for the electron. Transport calculations: Sn monolayer deposited on Au. (right) top view of the monolayer lattice commensurate with that of Au (111) surface.