Supplementary Information

Exploration of the Interaction Strength at the Interface of Neutral Chalcogen Ligands and Gold Surfaces

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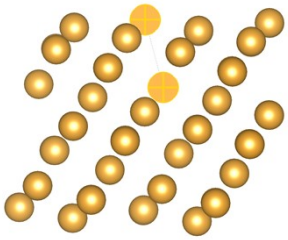
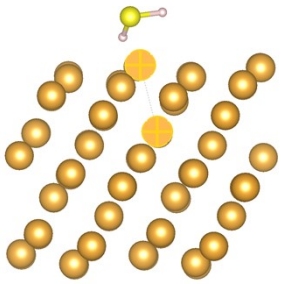
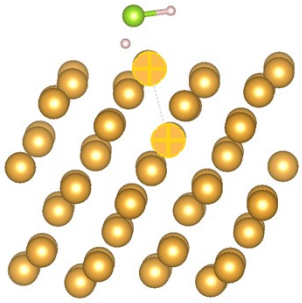
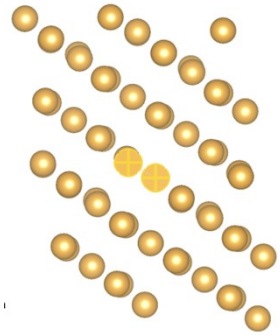
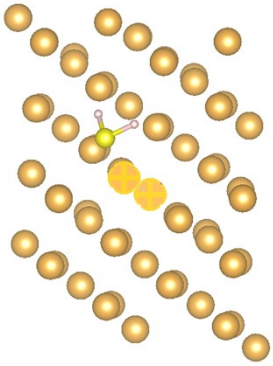
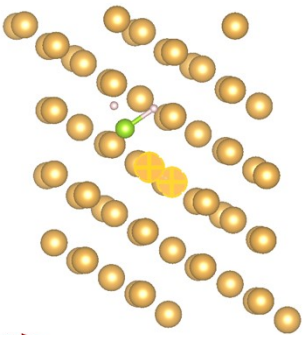
	Au-32$\bar{1}$ (Clean)	SH2- Au-32$\bar{1}$	SeH2- Au-32$\bar{1}$
Side view 			
Top view 			
d(Au-Au) Å	2.776	2.761	2.768
Δd Å	0.00	0.015	0.008

Figure S1. Side and top views of the clean Au-32$\bar{1}$ surface and the most stable adsorption geometries obtained for the XH_2 species (X = S, Se). The lower panel reports the average Au–Au distance in the surface layer together with the relaxation Δd relative to the clean slab. Adsorption induces only minimal structural distortion (Δd ≤ 0.02 Å), indicating that the stepped morphology of Au32$\bar{1}$ is largely preserved.

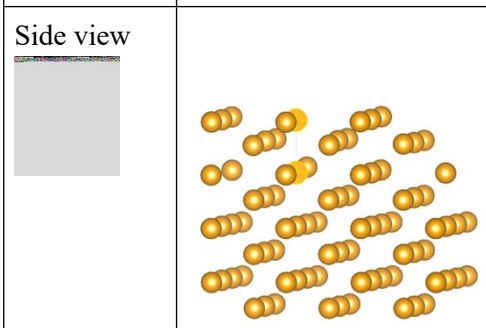
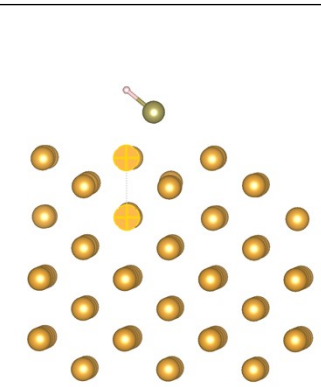
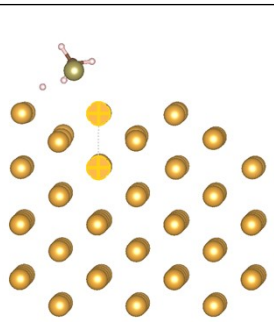
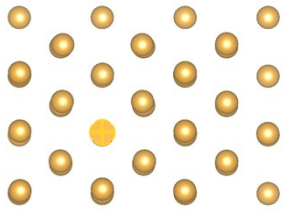
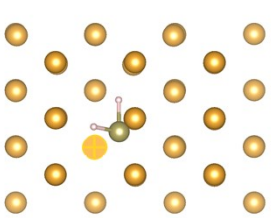
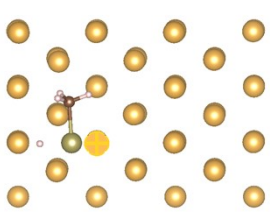
	Au-110 (Clean)	TeH2-Au110	TeHCH3-Au110
Side view			
Top view			
$d_{Au\text{-}Au}$ (Å)	2.830	2.859	2.873
Δd (Å)	0.00	0.029	0.043

Figure S2. Side and top views of the clean Au(110) surface and the most stable adsorption geometries obtained for TeH_2 and $TeHCH_3$. The lower panel summarizes the average surface Au–Au distances and the corresponding relaxation Δd relative to the clean slab. Adsorption of Te-containing species leads to somewhat larger distortions than those observed for S- and Se-containing adsorbates, with Δd ≈ 0.03–0.05 Å, while the characteristic row-like morphology of Au(110) remains essentially unchanged.

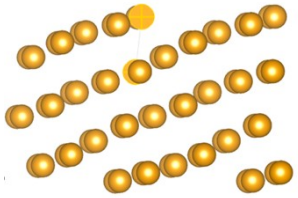
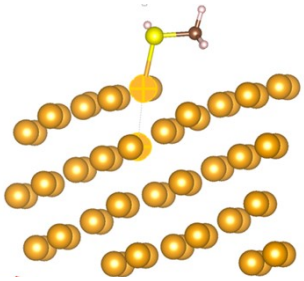
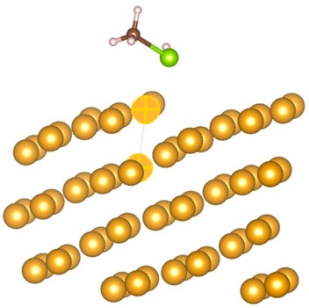
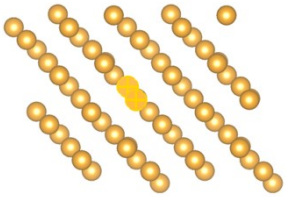
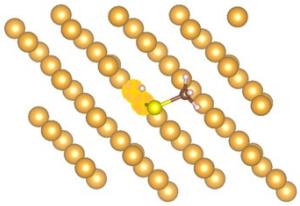
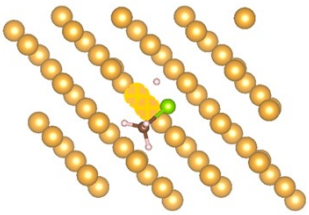
	Au-321 (Clean)	SHCH3-Au321	SeHCH3-Au321
Side view			
Top view			
d_{Au-Au} (Å)	2.775	2.723	2.718
Δd (Å)	0.00	0.052	0.057

Figure S3. Side and top views of the clean Au(321) surface and the most stable adsorption geometries obtained for the $XHCH_3$ species (X = S, Se). The lower panel reports the average Au–Au distance in the topmost layer and the relaxation Δd relative to the clean slab. Adsorption at step-edge Au atoms produces moderate but localized distortions (Δd ≈ 0.05 Å), consistent with the higher reactivity of high-index stepped facets.

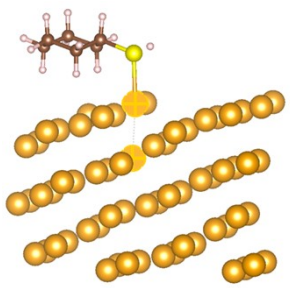
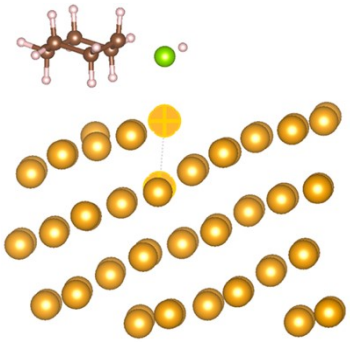
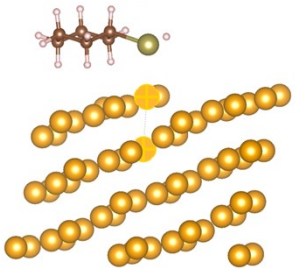
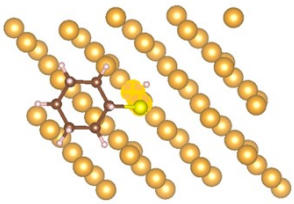
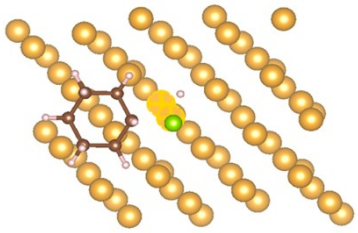
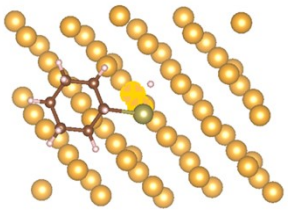
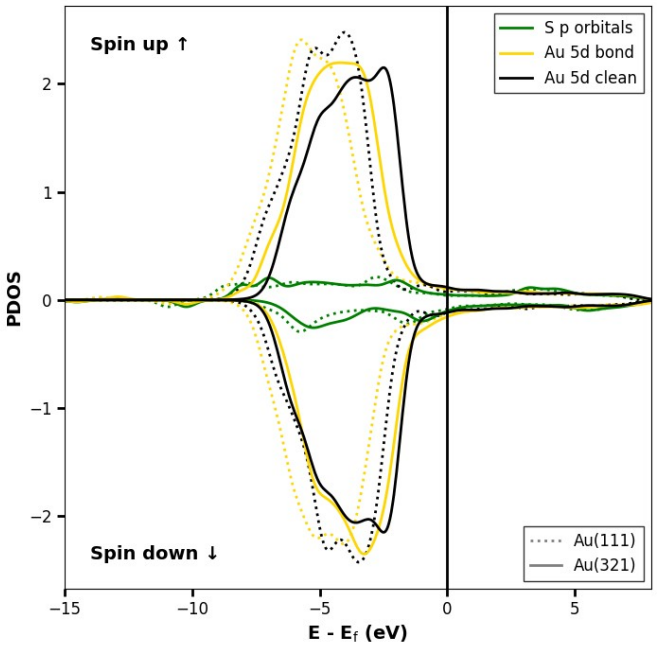
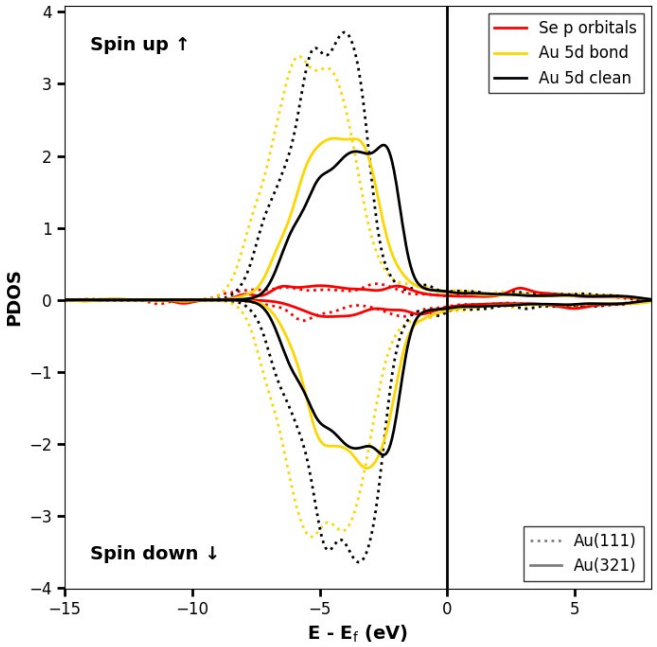
	SHC6H11-Au-321	SeHC6H11-Au321	TeHC6H11-Au321
Side view			
Top view			
d_{Au-Au} (Å)	2.736	2.729	2.733
Δd (Å)	0.039	0.046	0.042

Figure S4. Side and top views of the most stable adsorption geometries of the XC_6H_{11} species (X = S, Se, Te) on the Au(321) surface. The lower panel displays the average Au–Au distance in the surface layer and the corresponding relaxation Δd relative to the clean slab. The bulkier C_6H_{11} substituent enhances surface relaxation slightly (Δd ≈ 0.04–0.05 Å), though the stepped topology of Au(321) is maintained.

Table S1. Comparison between the total energies and adsorption energies obtained using the r²SCAN meta-GGA functional (with and without rVV10 dispersion correction) and those

calculated in this work using the GGA+D3 approach (IVDW=11). Two representative systems





ΔE		.469	71.6
Most Stable		t = 11	% Dis
Au321-$TeHC_6H_{11}$		)45848	
Au321		8771	
$TeHC_6H_{11}$		20562	
ΔE		5764	56.6

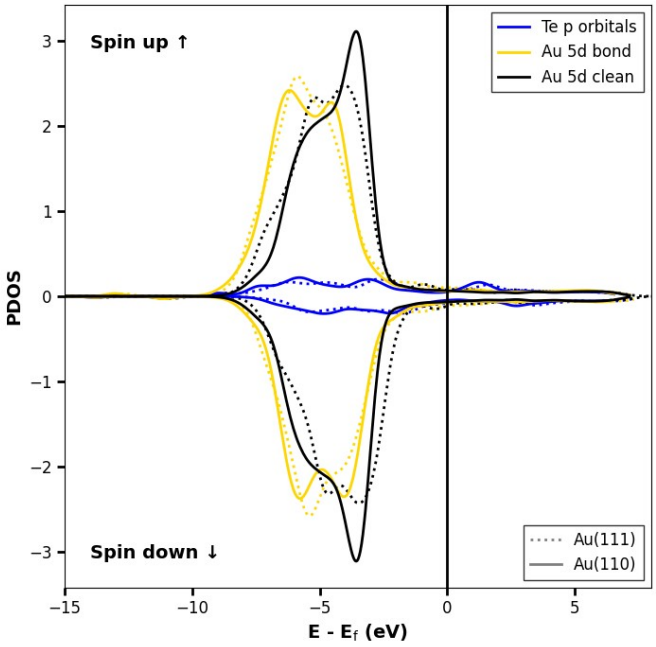


Figure S5: Spin-polarized projected density of states (PDOS) for systems $AuXHCH_3$ with chalcogen (X = S, Se, Te) p-orbitals and gold 5d-orbitals on clean and adsorbed surfaces.

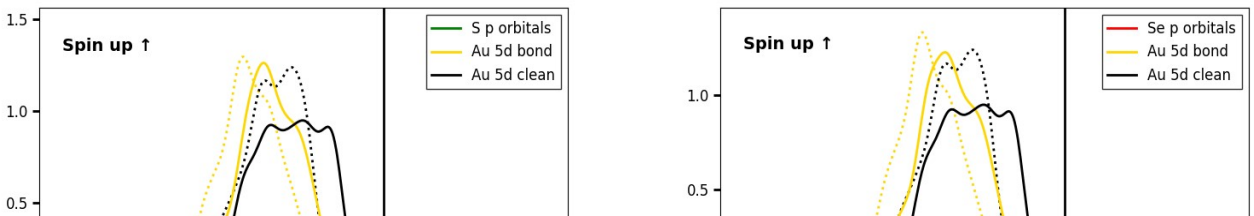


Figure S6: Spin-polarized projected density of states (PDOS) for systems $AuXHC_6H_{11}$ with chalcogen (X = S, Se, Te) p-orbitals and gold 5d-orbitals on clean and adsorbed surfaces.