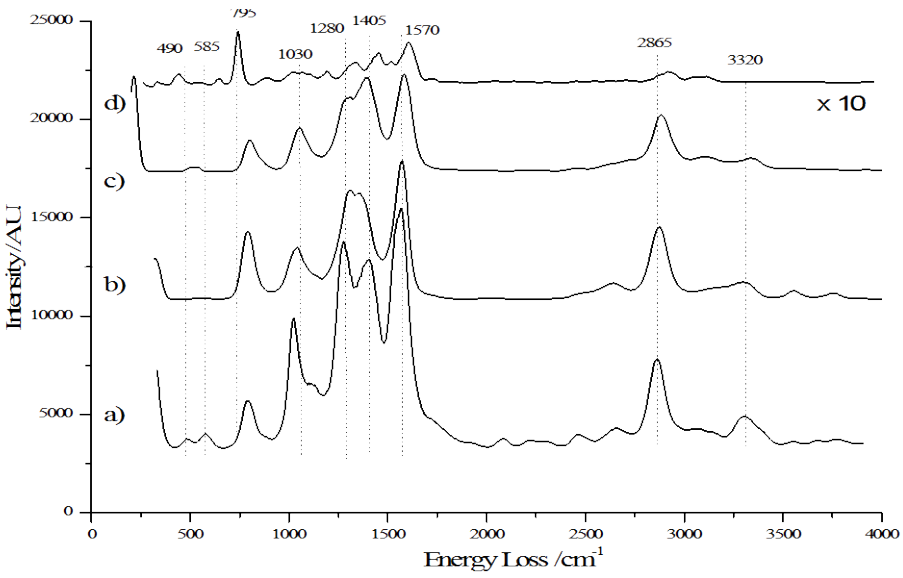
Supplementary Information

HREELS of lysine on Au{111} at 300 K



Energy loss /cm^{-1}

HREELS data are presented as a function of increasing annealing temperature following the adsorption of *(S)*-Lys on Au{111} a) 298 K, b) 333 K, c) 353 K and d) 373 K. It is clear that, by 373 K, almost all of the adsorbed lysine has desorbed from the surface. Adsorbed lysine exists mainly in the neutral form with some contribution from the zwitterionic form. The lack of a sizeable ν(C=O) feature at ~1700 cm^{-1} is presumably due to the carboxylic acid dimer being essentially parallel to the surface and therefore not observed due to the surface dipole selection rule.

HREELS /cm^{-1}	Assignment of bands[1]
Room Temperature	
3320	ν (NH_2)
2865	ν_{asym} CH_2
1570	δ NH_2
1405	ν_{sym} COO^-
1280	ν_{acid} C-OH
1030	ν (CN)
795	NH_2 wag
585	ν (Au-N)
490	ν (Au- N)

Table 1 Vibrational assignments of adsorption HREELS bands (in cm^{-1}) of *(S)*-lysine adsorbed onto Au{111}.

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DFT calculations of adsorption energy of a range of configurations of lysine on Au{111}

	Functional groups pointing towards surface	**dE in kJmol^{-1}**
Single lysine molecule	α-N, ε-N	-282.3
	COOH	-243.0
	COOH, ε-N	-271.8
zwitterion	COO, α-N	-217.2
lysine dimer	ε-N	-300.9
	COOH, ε-N	-295.7
	COOH	-288.6

The most stable form of lysine identified in the DFT calculations comprises a lysine dimer interacting with the surface via the ε-NH_2 functionality.

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Atomic co-ordinates of most stable lysine adsorption geometry

```
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  3   8 O
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%endblock AtomicCoordinatesAndAtomicSpecies

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References

1 V Humblot, C Methivier, and C M Pradier, *Langmuir*, 2006, **22**, 3089