Supplementary Information

The gold/ampicillin interface at the atomic scale

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Figure S1: Projected Density of States in the case of the "direct" adsorption of the protonated ampicillin on Au(110). In black: d states of an Au surface atom. In red: d states of the S-bonded Au surface atom. In blue: p states of the S atom.



Figure S2: Projected Density of States in the case of the "direct" adsorption of the protonated ampicillin on Au(110). In black: d states of an Au surface atom. In red: d states of the N-bonded Au surface atom. In blue: p states of the N atom.



Figure S3: Projected Density of States in the case of the "direct" adsorption of the deprotonated ampicillin on Au(110). In black: d states of an Au surface atom. In red: d states of the O-bonded Au surface atom. In blue: p states of the O atom.