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Title: The Effect of the Adsorbate Layer on the Work Function Reduction of Gold Substrates under External Electric Fields

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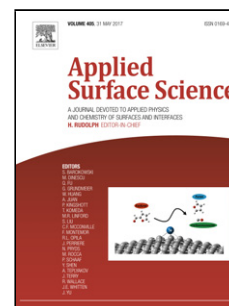
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## Highlights

(CH<sub>3</sub>)<sub>2</sub>S adsorption on Au(111) was calculated with density functional method.

The effect of electric field on (CH<sub>3</sub>)<sub>2</sub>S adsorption was examined.

The mechanism of the substrate work function reduction is theoretically explored.

The work function of Au gate sensitively correlates the content of (CH<sub>3</sub>)<sub>2</sub>S.

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