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Authors: Wenju Wang, Lili Fan, Guoping Wang

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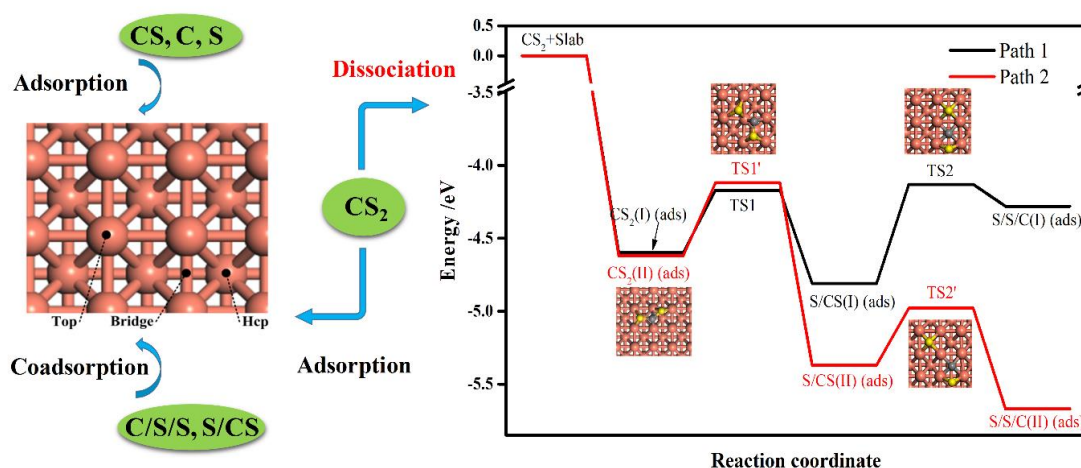
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# Carbon disulfide ( $\text{CS}_2$ ) adsorption and dissociation on the $\text{Cu}(100)$ surface: A quantum chemical study

Wenju Wang<sup>‡</sup>, Lili Fan, Guoping Wang<sup>§</sup>

School of Energy and Power Engineering, Nanjing University of Science and Technology, Nanjing 210094, China

## Graphical Abstract



## Highlights

- 1)  $\text{CS}_2$ , CS, C and S are strongly chemadsorbed on the  $\text{Cu}(100)$  surface.
- 2) C/S/S, S/CS and  $\text{CS}_2$  accord to a decreased adsorption strength on the  $\text{Cu}(100)$ .
- 3) The asymmetric model  $\text{CS}_2(\text{II})$  is easier to dissociate on the  $\text{Cu}(100)$  surface.

**Abstract:** Density functional theory (DFT) is used to examine the adsorption and dissociation of  $\text{CS}_2$  on the  $\text{Cu}(100)$  surface. This study evaluates the adsorption energies and geometries of the species ( $\text{CS}_2$ , CS, C and S) adsorption on the  $\text{Cu}(100)$  surface, as well as that coadsorption of CS and a S atom, and that coadsorption of C atom and two S atoms. The results indicate that the species ( $\text{CS}_2$ , CS, C and S) are strongly chemadsorbed on the  $\text{Cu}(100)$  surface through the C–Cu and/or S–Cu bond with an increased adsorption energy ( $\text{C/S/S} > \text{S/CS} > \text{CS}_2$ ). Two pathways for  $\text{CS}_2$

<sup>‡</sup> Corresponding author. E-mail address: wangwenju1982@gmail.com;

<sup>§</sup> Corresponding author. E-mail address: wgp1976@163.com

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