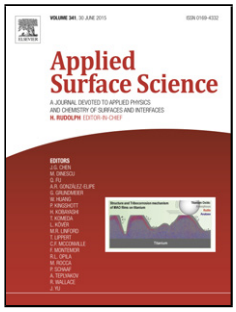

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Carbon disulfide (CS_2) adsorption and dissociation on the Cu(100) surface: A quantum chemical study

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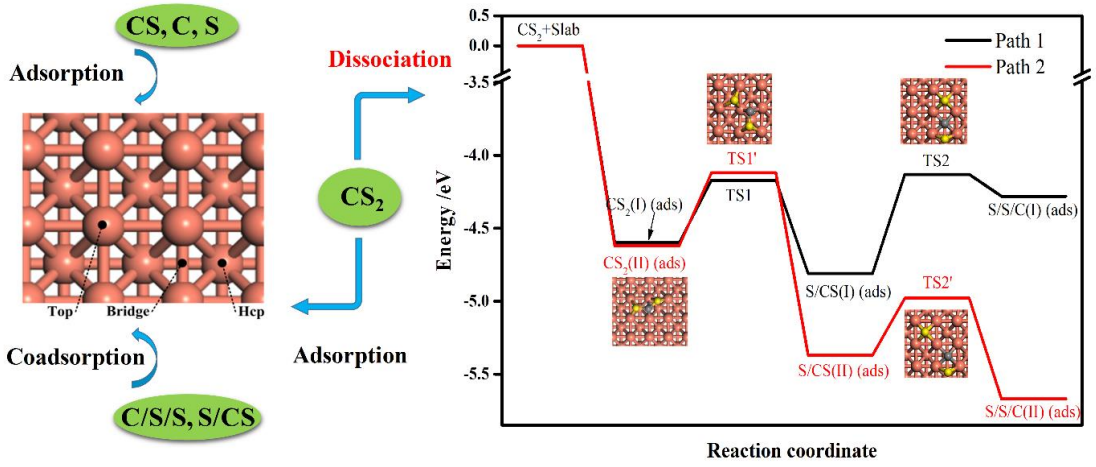
Graphical Abstract



Highlights

- 1) CS_2, CS, C and S are strongly chemadsorbed on the Cu(100) surface.
- 2) C/S/S, S/CS and CS_2 accord to a decreased adsorption strength on the Cu(100).
- 3) The asymmetric model CS_2(II) is easier to dissociate on the Cu(100) surface.

Abstract: Density functional theory (DFT) is used to examine the adsorption and dissociation of CS_2 on the Cu(100) surface. This study evaluates the adsorption energies and geometries of the species (CS_2, CS, C and S) adsorption on the 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 (CS_2, CS, C and S) are strongly chemadsorbed on the Cu(100) surface through the C–Cu and/or S–Cu bond with an increased adsorption energy (C/S/S>S/CS>CS_2). Two pathways for CS_2

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