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Cysteine and cystine adsorption on FeS_2(100)

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Highlights

- Sulfur-deficient surfaces play an important role in the adsorption of cysteine and cystine.
- In the thiol headgroup adsorption on the sulfur-vacancy site, dissociative adsorption is found to be energetically favorable compared with molecular adsorption.
- In the cystine adsorption on the defective surface under vacuum conditions, the formation of the S–Fe bond is found to be energetically favorable compared with molecular adsorption.
- Raman spectroscopic measurements suggest the formation of cystine molecules through the S–S bond on the pyrite surface in aqueous solution.

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