Accepted Manuscript

Title: Molecular-level insights into mercury removal mechanism by pyrite

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PII: S0304-3894(17)30760-4
DOI: https://doi.org/10.1016/j.jhazmat.2017.10.011
Reference: HAZMAT 18916

To appear in: *Journal of Hazardous Materials*

Received date: 14-7-2017
Revised date: 30-9-2017
Accepted date: 4-10-2017

Please cite this article as: Yingju Yang, Jing Liu, Feng Liu, Zhen Wang, Sen Miao, Molecular-level insights into mercury removal mechanism by pyrite, Journal of Hazardous Materials https://doi.org/10.1016/j.jhazmat.2017.10.011

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ACCEPTED MANUSCRIPT

Molecular-level insights into mercury removal mechanism by pyrite

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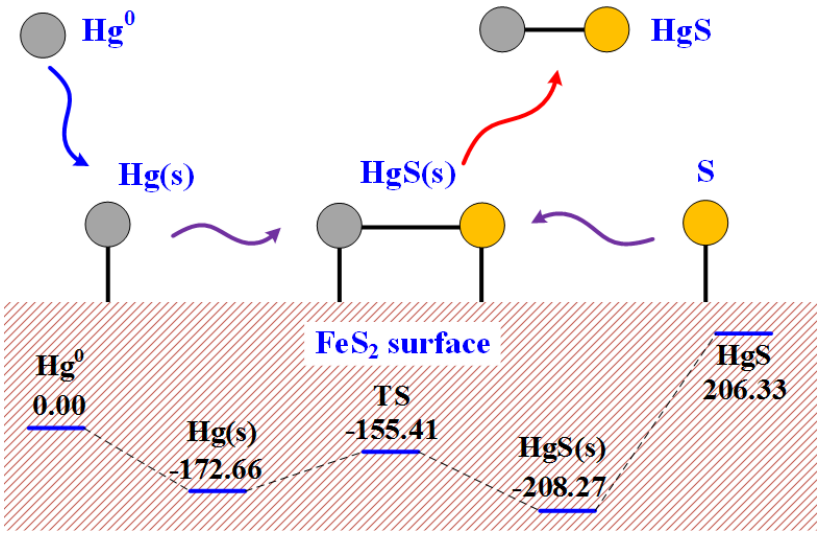
Graphical abstract



Highlights

- Surface reaction chemistry of Hg oxidation over FeS_2 was studied using DFT method.
- FeS_2(110) surface is much more active for Hg^0 adsorption than FeS_2(100) surface.
- The reaction pathway of heterogeneous Hg transformation is a three-step process.
- HgS desorption from FeS_2 surface is the rate-determining step.

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