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Research on Inhibitors and Hindered Groups in Ultra-deep Hydrodesulfurization Based on Density Functional Theory

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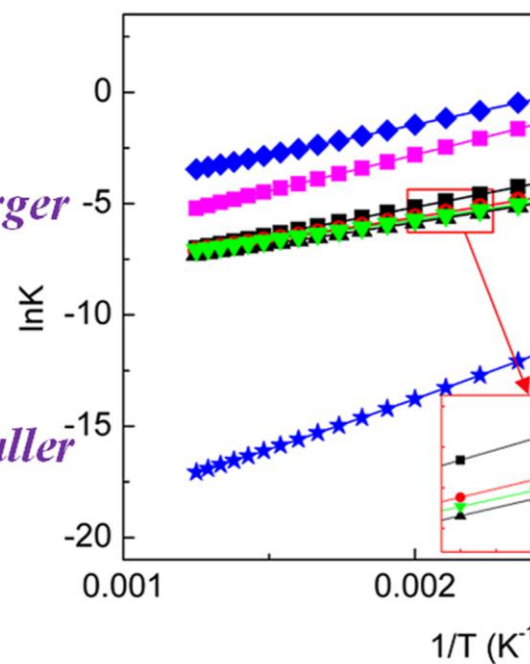
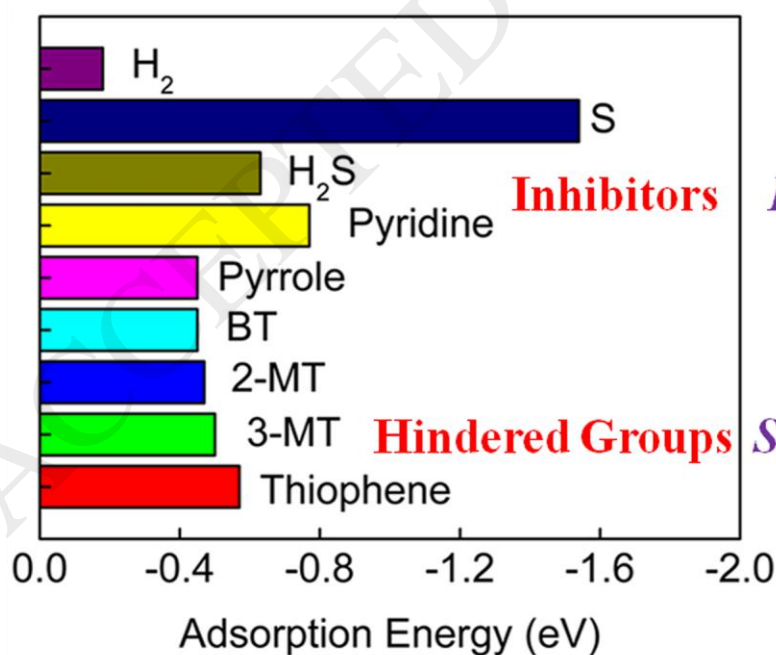
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Highlights

- Essence of effects of inhibitors and hindered groups on ultra-deep HDS is proposed.
- Inhibitors compete with sulfur compounds to adsorb to Ni₂P surface.
- Inhibitors weaken the interaction of thiophene with Ni₂P.
- Sulfur compounds adsorb to Ni₂P surface through Ni-S bonds.
- Hindered groups weaken the interaction of sulfur compounds with Ni₂P.

Graphical abstract



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