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Crossing-link of Experimental Reducibility Tests, XPS Characterizations and DFT Estimates on Ferrite Oxygen Carriers in CLC

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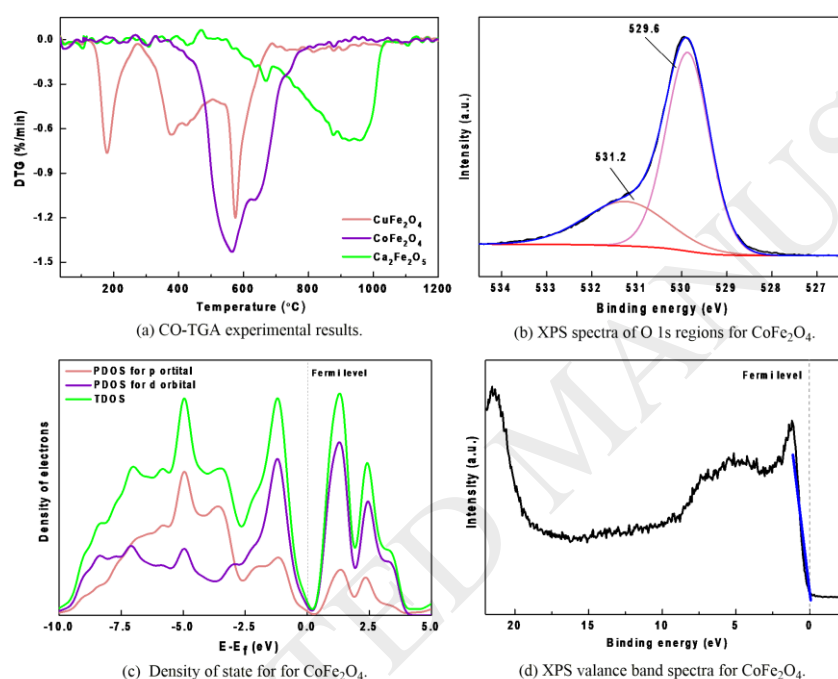
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Graphical abstract



A unique approach was applied to address general principles of selection on a series of ferrites as oxygen carriers.

Highlights

- Proportions of the lattice oxygen and Fe²⁺ in ferrites positively and negatively influence their reduction reactivity, respectively.
- Varieties of oxygen components in ferrites determine their reduction behaviors, such as reduction temperatures and reactivity.
- Both the extents of the O-2p and M-3d valance bands to Fermi level of ferrites positively influence their initial reducing temperature and the reduction rate, respectively.
- The prediction on the reducibility of ferrite materials is possible based on XPS characterizations and DFT calculations.

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