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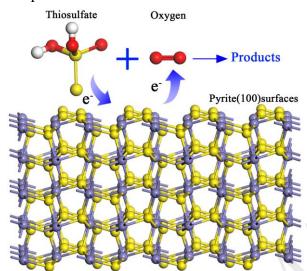
The catalytic decomposition of thiosulfate by pyrite

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Graphicl abstract



Rate-limiting step: the electron accepting process of oxygen

Highlights

- Donor impurities in pyrite can increase thiosulfate consumption on pyrite surfaces.
- Density functional theory (DFT) research results show that Co or Ni impurities increase the O-O bond length on pyrite surfaces.
- The rate-limiting step is the electron accepting process of oxygen during thiosulfate decomposition on pyrite surfaces.

Abstract: The rate-limiting step during catalytic decomposition of thiosulfate by pyrite was studied in detail in this paper. The results show that Co and Ni impurities in synthetic pyrite increase thiosulfate decomposition, but F impurities in synthetic pyrite reduce thiosulfate decomposition. Density functional theory (DFT) showed that Co and Ni impurities increase the pyrite (100) surface Fermi energy and reduce its

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