

Abstract Submitted
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Effect of annealing conditions on the healing of sulfur vacancy in pyrite FeS₂(100) surfaces¹ AMANDA WEBER, Department of Chemistry and Department of Chemical Engineering and Materials Science, University of California, Irvine, California 92697, YANNING ZHANG, Department of Physics and Astronomy, University of California, Irvine, CA 92697, NICHOLAS BERRY, MATTHEW LAW, Department of Chemistry and Department of Chemical Engineering and Materials Science, University of California, Irvine, California 92697, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, CA 92697 — Through density functional calculations, we investigated the segregation of a sulfur vacancy from interior sites outward to the FeS₂(100) surfaces in different surface conditions in order to provide guidance for the development of iron pyrite in photovoltaics applications. We found that the surfaces with interior S-vacancy are energetically unstable and bulk S-vacancies tend to hop toward the surface, in particular when the surface composition is in the stoichiometric or S-rich side. The segregation process is accompanied by redox reaction near the vacancy site, $\text{Fe}(2+) + \text{S}(1-) \rightarrow \text{Fe}(3+) + \text{S}(2-)$, and the activation energy decreases near the surface region. We compare the calculated structural, energetic and electronic properties to experimental data, and provide insights for reduction of vacancy density in optimal annealing conditions.

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