

Abstract Submitted  
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**Oxygen vacancy formation in doped ceria: Effects of electron localization and ion local distortion**<sup>1</sup> ZHENPENG HU, Nankai University — Density functional theory with plus U approximation has been used to study property of doped ceria, especially oxygen vacancy formation energy on doped CeO<sub>2</sub> surface. Surfaces with substitutional dopants having lower valence than Ce(IV) have been studied in detail. Based on our results, there are two factors affecting the formation energy of oxygen vacancy: electron localization to form polaron, and local distortion around dopant while vacancy generating. We discuss related application for these rules in catalysis process.

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Zhenpeng Hu  
Nankai University

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