Density Functional Theory Study of Gas Adsorption on Lanthanum Zirconate Nanostructured Coating Surface

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Lanthanum zirconate (La₂Zr₂O₇) is a typical pyrochlore ceramic material, which can be used as thermal barrier coating (TBC). However, it may deteriorate by oxidizing and corrosive gases, such as CO₂, O₂, SO₂ and CH₄ during its operation process at elevated temperatures. This work investigates CO₂, O₂, SO₂ and CH₄ gas adsorption mechanism on La₂Zr₂O₇ nanostructured coating surfaces using the density functional theory (DFT) calculations. La₂Zr₂O₇ surface energies on (001), (011) and (111) planes were calculated. Results show the most thermodynamically stable surfaces of La₂Zr₂O₇ are (011) and (111) planes, due to their low surface energies. Adsorption energies of CO₂, O₂, SO₂ and CH₄ on (001), (011) and (111) planes in different sites were studied as well. The results show the most favorable gas adsorption sites for CO₂, O₂, SO₂ and CH₄ occur at 3-fold and 4-fold sites. The most favorable gas adsorption plane for CO₂, O₂, SO₂ and CH₄ is (111) plane.