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# The Effects of Oxygen Partial Pressure to the Anti-Corrosion Layer in the Liquid Metal Coolant: A Density Functional Theory Simulation

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**Abstract :** The lead-bismuth eutectic (LBE) alloy is a promising candidate of coolant in the fast neutron reactors and accelerator-driven systems (ADS) because of its good properties, such as low melting point, high neutron yields and high thermal conductivity. Although the corrosion of the structure materials caused by the liquid metal (LM) coolant is a challenge to the safe operating of a lead-bismuth eutectic nuclear reactor. Thermodynamic theories, experiential formulas and experimental data can be used for explaining the maintenance of the protective oxide layers on stainless steels under satisfaction oxygen concentration, but the atomic scale insights of such anti-corrosion mechanisms are little known. In the present work, the first-principles calculations are carried out to study the effects of oxygen partial pressure on the formation energies of the liquid metal coolant relevant impurity defects in the anti-corrosion oxide films on the surfaces of the structure materials. These approaches reveal the microscope mechanisms of the corrosion of the structure materials, especially for the influences from the oxygen partial pressure. The results are helpful for identifying a crucial oxygen concentration for corrosion control, which can ensure the systems to be operated safely under certain temperatures.

**Keywords :** oxygen partial pressure, liquid metal coolant, TDDFT, anti-corrosion layer, formation energy
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