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First Principles Study of α -U₂N₃ Surfaces and its Anti-oxidant Mechanism MENGTING JIN, YANNING ZHANG, Chengdu Green Energy and Green Manufacturing Technology RD Center — With the advantages over oxides as fuel materials for fast nuclear reactors, actinide nitrides have been extensively studied in experiments. In particular, α -U₂N₃ is also the main composition of surface layer obtained by surface nitriding for the enhancement of oxidation resistance of uranium in ambient conditions.[1-4] However, the anti-oxidant mechanism behind is still unclear, which hinders the further development of surface treatment technologies for uranium. Here we perform extensive ab initio studies on the geometric, magnetic and electronic properties of α -U₂N₃ bulk and (001) surfaces. Then the adsorption and diffusion of O₂ near the stable α -U₂N₃(001) surface will be discussed, focusing on the local atomic arrangements of U-N and U-N-O that cannot be observed easily in experiments. Our theoretical results may give some insights in understanding the anti-oxidant mechanism of surface nitriding.

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