

炼铝用碳阳极中碱金属氧化物作用机理的量子化学研究

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摘要 本文应用CNDO/2法研究了炼铝用碳阳极中添加碱金属氧化物的吸附行为,通过优化得到了吸附的最佳模型,考察了吸附结合能随分子间距的变化,进而给出了碱金属氧化物在碳阳极中作用的机理。量子化学计算结果表明:碱金属氧化物添加到炼铝用碳阳极中起传输电子的电桥作用,是碳阳极在空气中氧化反应以及铝电解时生成氧气的氧化反应的催化剂;理论计算和实验结果二者吻合较好,可以用来解释若干实验结果。

关键词 [吸附](#) [氧化物](#) [微分重叠全忽略近似](#) [碱金属化合物](#) [碳阳极](#)

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Quantum chemical study on the mechanism of alkaline metal oxide in carbon anode for aluminum electrolysis

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Abstract In this paper the absorption performance of alkaline metal oxide in carbon anode for aluminum electrolysis was studied by CNDO/2 method. The best model is obtained by optimizing in calculation of total energy and binding energy. It was found that the absorption total energy and binding energy varied with the molecular distance. The calculation result shows that the carbon anode can absorb alkaline metal oxide. After being absorbed, the alkaline metal oxide can absorb oxygen, which may be a chemical absorption. The alkaline metal oxide in carbon anode for aluminum electrolysis plays a role of transmitting electrons and acts as one kind of catalyst for the oxidation reaction. The theoretical calculation results are in good agreement with the experimental ones. Reports referring to the effect of alkaline metal oxide in carbon anode by CNDO/2 method have not yet been found at present time.

Key words [ADSORPTION](#) [OXIDE](#) [CNDO APPROXIMATION](#) [ALKALI METAL COMPOUNDS](#)

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