Chemisorption of oxygen and subsequent reactions on low index surfaces of β-Mo2C - DTU Orbit (28/12/2018)

Chemisorption of oxygen and subsequent reactions on low index surfaces of β-Mo2C: Insights from first-principles thermodynamics and kinetics

Oxygen chemisorption on β-Mo2C surfaces, the subsequent CO/CO2 desorption and oxygen diffusion to the carbon vacancy have been investigated by density-functional theory. The most stable structures together with the energetics of oxygen stepwise adsorption, CO/CO2 desorption and oxygen diffusion to the carbon vacancy were identified. We examined the effect of oxygen coverage on the morphology of β-Mo2C by plotting the equilibrium crystal shape. Thermodynamic effect of temperature and reactant or product pressure on the CO/CO2 desorption were investigated. The CO/CO2 desorption is more favorable at the saturated oxygen coverage than the low oxygen coverage thermodynamically. The subsequent oxygen diffusion to the carbon vacancy after CO/CO2 desorption may happen depending on the surfaces and oxygen coverage.

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