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Study of higher tungsten boride for catalytical application

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Nowadays the most widely used catalysts for organic synthesis mainly made of noble and rare earth metals that significantly increases the cost of many products. Moreover, 80% of catalyst used in domestic industry including oil and chemical production are imported and it can cause problems in the present political situation.
Suggested alternative to the pricey catalysts is the transition metals borides [1], [2]. Along with the other transition metal borides, tungsten borides were studied as potential catalysts for hydrogen evolution reaction (HER) and CO₂ conversion to CH₄, then, their usage as the catalysts for organic synthesis was proposed.
Furthermore, as it was showed for Mo-B system [3], the catalytic activity of transition metal borides increases with the boron stoichiometric content. Hence, the higher tungsten boride (WB_{5-x}) is the most promising one beyond the other tungsten borides.
Here we performed the comprehensive study of surfaces of WB_{5-x} using density functional theory (DFT) as implemented in VASP package. We studied the surface energies of WB_{5-x} slabs with (001), (010), (100), (110), (101), (111), (130), and (201) crystallographic orientations. Calculated surface energies were used to make Wulff construction by using Python WulffPack module to find the equilibrium morphology of higher tungsten boride single crystal. It was shown that boron terminated (010) and (001) surfaces and tungsten terminated (101) surface are the most stable.
As WB_{5-x} has also proposed as the alternative to the catalysts for an automotive motor, the adsorption of the different atmosphere gases (CO, CO₂, H₂, N₂, O₂, NO, NO₂, H₂O, NH₃, SO₂) on its stable surfaces was investigated. It was shown that at the (010) surface the lowest adsorption energies have the NO, CO and H₂ molecules. On the contrary, WB_{5-x} surface doesn't adsorb SO₂ gas. On (101) surface O₂, NH₃ and NO₂ have the lowest adsorption energies. It is worth noting, that O₂ molecule easily dissociates o both of considered surfaces.
Obtained results allows us to possess higher tungsten boride as a perspective catalyst or co-catalyst for many different reactions including photocatalytical ones. Furthermore, the experimental work to prove data obtained is already started.

References:
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