Scaling Relations on Basal Plane Vacancies of Transition Metal Dichalcogenides for CO2 Reduction - DTU Orbit (18/08/2019)

Scaling Relations on Basal Plane Vacancies of Transition Metal Dichalcogenides for CO2 Reduction

Transition metal dichalcogenides (TMDs) have shown promising electrocatalytic performance for CO2 reduction (CO2R) recently. However, the development of efficient and selective catalysts remains a major challenge. While recent studies have suggested the importance of activation energies as activity descriptors for CO2R beyond CO, the scaling of intermediate binding energies present a first step in computational catalyst screening. Here, we investigate the basal vacancy on 2H and 1T/1T' phase group V, VI and X TMDs for CO2R reduction. We find that the change of oxophilicity and carboxophilicity on each group of TMDs follow different trends, which leads to different scaling relations amongst key intermediates. Our thermochemical analysis also suggests Group V and VI TMDs to be either selective for hydrogen evolution reaction (HER) or prone to OH poisoning. However, the initial analysis suggests group X TMDs to be possible candidates for active and selective CO2R reduction without suffering from OH poisoning, which motivates further theoretical kinetic studies. We furthermore find that their reaction energetics can be tuned by the density of the basal vacancies.

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