Scaling Relations on Basal Plane Vacancies of Transition Metal Dichalcogenides for CO2 Reduction - DTU Orbit (26/02/2019)

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/1'T phase group V, VI and X TMDs for CO2R reduction. We find that the change of oxophilicity and carbophilicity 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.

General information
State: Published
Organisations: Department of Physics, SLAC National Accelerator Laboratory
Contributors: Ji, Y., Nørskov, J. K., Chan, K.
Number of pages: 6
Pages: 4256-4261
Publication date: 2019
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry C
Volume: 123
Issue number: 7
ISSN (Print): 1932-7447
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
Web of Science (2017): Impact factor 4.484
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195
Web of Science (2016): Impact factor 4.536
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4.68 SJR 1.886 SNIP 1.26
Web of Science (2015): Impact factor 4.509
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 5.08 SJR 2.032 SNIP 1.447
Web of Science (2014): Impact factor 4.772
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 5.14 SJR 2.143 SNIP 1.445
Web of Science (2013): Impact factor 4.835
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 4.98 SJR 2.529 SNIP 1.461
Web of Science (2012): Impact factor 4.814
ISI indexed (2012): ISI indexed yes