

(Abstract 7)

## "Revealing the role of the 1T phase on the adsorption of organic dyes on MoS<sub>2</sub> nanosheets"

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## Abstract

Herein, different phases of  $MoS_2$  nanosheets were synthesized, characterized and tested for dye removal from water. The influence of the  $MoS_2$  phases as well as the 1T concentration on the adsorption performance of organic dyes MO, RhB and MB was deeply investigated. The results revealed that the 1T-rich  $MoS_2$  nanosheets have superior adsorption performance compared to other 2H and 3R phases. The kinetic results of the adsorption process demonstrate that the experimental data followed the pseudo-second order equation. Meanwhile, the adsorption of dyes over the obtained materials was fitted with several isotherm models. The Langmuir model gives the best fitting to the experimental data with maximum a adsorption capacity of 787 mg g<sup>-1</sup>. The obtained capacity is significantly higher than that of all previous reports for similar  $MoS_2$  materials. Computational studies of the 2H and  $1T/2H-MoS_2$  phases showed that the structural defects present at the 1T/2H grain boundaries enhance the binding of hydroxide and carboxyl groups to the  $MoS_2$  surface which in turn increase the adsorption properties of the  $1T/2H-MoS_2$  phase.