

MRS Fall 2024

## View Abstract

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<b>ABSTRACT</b>
<b>TITLE:</b> Improving Monolayer MoS <sub>2</sub> Optical Properties Through Thermal Treatments
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<b>ABSTRACT BODY:</b> <b>Abstract Body:</b> The research on two dimensional (2D) materials has recently witnessed rapid advancements towards industrial applications. In particular, several efforts have been poured into the development of optoelectronic devices based on heterostructures composed of several stacked 2D layers having complementary features.[1] Van der Waals materials such as semiconducting transition metal dichalcogenides (TMDs) are considered particularly useful for their atomic-scale thickness, direct bandgap, and good electronic and mechanical properties.[2] Among these, monolayer molybdenum disulphide (1L-MoS <sub>2</sub> ) has been widely studied so that nowadays several different production routes which can be easily scaled up and allow to obtain flakes of large size and high quality are available. The intense photoemission at 1.8eV displayed by 1L-MoS <sub>2</sub> flakes excited in the visible light range, originating from an excitonic recombination, is strongly coupled to properties of the material such as strain and doping.[3] Consequently, defects introduced in the monolayer structure during the synthesis can significantly affect the optical performances of this material.[4] Nonetheless, it is possible to exploit the high sensitivity of 1L-MoS <sub>2</sub> to the external environment in order to enhance its photoluminescence by modifying its structural properties following its production. We have explored how performing thermal treatments conducted under a controlled atmosphere allows to predictably alter the properties of this 2D semiconductor, affecting its strain and doping while at the same time tuning the shape and intensity of its emission. We have compared several 1L-MoS <sub>2</sub> flakes obtained using different preparation methods and studied their properties before and after each thermal treatment. Additionally, in order to better understand the underlying mechanism, the effect of different atmospheres used to perform the treatments has been compared while observing at the same time how the physical properties of conducting, insulating or semiconducting substrates can have a role in the overall results. In general we were able to observe an enhancement of the optical properties of the studied 1L-MoS <sub>2</sub> , indicating the effectiveness of the post-synthesis procedure towards reducing the defects introduced by some preparation methods. As such, we believe that our results allow to make use of the most advantageous production routes by solving their drawbacks through an

additional treatment step. From a fundamental perspective, the performed comparison enables us to further understand the role of the several factors influencing the optical properties of 1L-MoS<sub>2</sub> and to attempt to harness them. Finally, we aim to control the light-emitting capabilities of the studied 2D material towards its usage in the field of optoelectronics, exploiting the developed post-synthesis treatments versatility for the realization of heterostructure-based devices incorporating 1L-MoS<sub>2</sub> flakes. The Italian MUR PNRR project SAMOTHRACE (ECS00000022) and the Italian MUR PRIN 2022 project 2DIntegratE (2022RHRZN2) are gratefully acknowledged.

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