Sub-nanometric MoOx clusters arising on single MoS2 flakes due to oxidative etching at elevated temperatures.

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 Layered semiconductor MoS2 as a representative of transition metal dichalcogenides (TMDs) family has been used in (opto)electronic and energy-harvesting devices due to its fascinating properties. In order to improve its properties or predict their device performances, any surface reaction, in particular oxidation, of MoS2 flakes is of great importance [1]. In this contribution, presence of small oxide clusters on heated single MoS2 flakes will be discussed. First, high resolution non-contact and contact atomic force microscopy (AFM) images form such flakes are presented to detect surface distribution and height profiles of the oxide clusters. The height histogram of 1000+ loosely-surface-bound clusters shows two peaks at 0.236 ± 0.006 nm and 0.472 ± 0.021 nm, respectively [2]. Density Functional Theory (DFT) simulations on the sub-nanometric MoxOy fragments onto a MoS2 monolayer were done to shed light on chemical composition of such clusters. Based on AFM and DFT simulation results, such clusters were attributed to MoO3 monomers and dimers arising from single oxidative etching events on the thermally treated single MoS2 flakes [1,2].

1. R. Szoszkiewicz, Local Interactions of Atmospheric Oxygen with MoS2 Crystals. Materials, 2021, 14(20), p.5979.
2. S. Sovizi, S. Tosoni, R. Szoszkiewicz, MoS2 oxidative etching caught in the act: Formation of single (MoO3)n molecules, under review, Chemical Communications.