

Ph.D. Course in Materials Science and Nanotechnology

University of Milano-Bicocca, Department of Materials Science, via R. Cozzi 55, 20125 Milano

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Seminar room - Department of Materials Science U5

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Interactions of oxygen with MoS₂ crystals investigated at microscopic length scales.

For numerous applications of microscopic MoS₂ crystals, particularly in flexible nanoelectronics, one must understand their oxidation reactions in air and water [1]. In this seminar, I will present some case studies of microscopic heat induced oxidation and oxidative etching performed on thick, mechanically exfoliated, geological 2H MoS₂ crystals in air. I will discuss some particular reaction mechanisms and our efforts in detecting various forms of MoO₃ oxides onto such surfaces. In order to do so, we combined various global and local measurements such as XPS, XAS, Raman and AFM (topography, friction, Kelvin Probe) on single microscopic MoS₂ flakes [2,3]. To have a closer look into an atomistic level at one particular oxidation regime, we combined experimental results with DFT calculations, which have been performed by prof. Sergio Tosoni at University of Milan-Bicocca.

[1] R. Szoszkiewicz, Local interactions of atmospheric oxygen with MoS₂ crystals, *Materials*, 14, 5979, 31 pages (2021).

[2] M. Rogala, S. Sokołowski, U. Ukegbu, A. Mierzwa and R. Szoszkiewicz, Direct identification of surface bound MoO₃ on single MoS₂ flakes heated in dry and humid air, *Advanced Materials Interfaces*, 2100328, 11 pages (2021);

[3] S. Sovizi, S. Tossoni, R. Szoszkiewicz, "Caught in the act": formation of single (MoO₃)_n molecules within basal MoS₂ planes during their oxidative etching, *Nanoscale Advances* (2022) DOI: 10.1039/d2na00374k

PhD students and all interested in the seminar are kindly invited to participate.

The PhD Coordinator
Prof. Marco Bernasconi