Namur Institute of Structured Matter

UNIVERSITÉ DE NAMUR

NISM Seminar

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« Defects related properties in two-dimensional MoS_2: Experiment and Theory »

When and where:

Wednesday October 9th 2019 at 16:00
UNamur, Rue Grafé 2, B-5000 Namur
Chemistry & Physics building
Auditorium CH21 (2nd floor)

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« Defects related properties in two-dimensional MoS_2: Experiment and Theory »

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The presence of defects in 2D materials can significantly influence the electronic, magnetic or optical properties of the material with a direct impact on applications. In this seminar we provide atomic level insights into the properties of point defects (0D) and line defects (1D) of single layers MoS_2 by using electronic structure calculations combined with atomic resolution Scanning Tunneling Microscopy (STM) measurements. We found that under ambient conditions oxygen gradually incorporates into the basal plane of the MoS_2 crystals through a substitutional oxidation reaction, by replacing individual sulfur atoms [1]. These point defects can be identified as active reaction centers, increasing the catalytic activity for electrochemical H_2 evolution reaction. The possibility to modify the structure by individual heteroatoms has a key importance for understanding the structure−activity relationship at the atomic scale, such as the contribution of the heteroatoms and neighboring host atoms to the catalytic process [2]. In the case of the line defects, we have investigated the magnetic properties of zigzag edges of several nanometer long MoS_2 nanoribbons by using the Hubbard model [3]. In contrast to graphene nanoribbons, our results predict low domain wall energies along the edges, which are also sensitive to the presence of edge disorder. Our theoretical and experimental results give an insight into the properties of defects in MoS_2 and can also provide valuable information for catalytic and spintronic applications.

References

[1] J. Pető, T. Ollár, P. Vancsó et al., *Nat. Chem.* **10**, 1246–1251 (2018).
[2] P. Vancsó, Z. I. Popov, J. Pető et al., *ACS Energy Lett.* **4**, 1947−1953 (2019).
[3] P. Vancsó, I. Hagymási, P. Castenetto et al., *Phys. Rev. Mater.* **3**, 094003 (2019).