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Synthesis of epitaxial monolayer Janus SPtSe

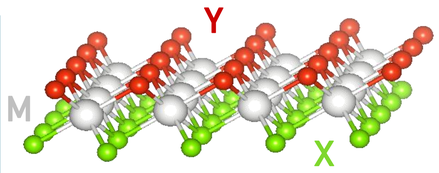
Roberto Sant*, M. Gay, A. Marty, S. Lisi, R. Harrabi, C. Vergnaud, M. T. Dau, X. Weng, J. Coraux, N. Gauthier, O. Renault, G. Renaud, M. Jamet

* ESRF, the European Synchrotron, 38043 Grenoble, France

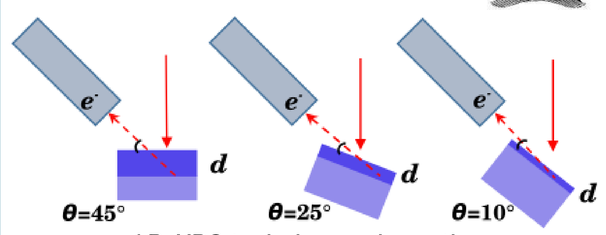
Janus Transition Metal Dichalcogenides (TMDCs)

Monolayer TMDCs whose chalcogen layers are of different chemical nature (e.g. **XMY, M=metal, X=Se and Y=S**) are said **Janus** after the **biface** Roman god[1]. They can be prepared by selectively substituting the chalcogen atoms in the pristine TMDC topmost layer by annealing the material in a suitable gaseous precursor atmosphere of another chalcogen species. It turns out that the vertical mirror symmetry in the Janus TMDC is broken.

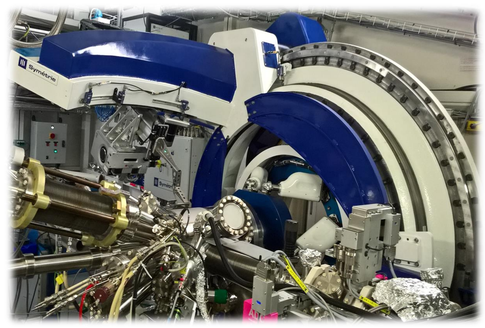
By *operando in situ* grazing incidence X-ray diffraction (**GIXRD**) at the BM32 beamline at ESRF, we could follow the structural transformation of a TMDC into a Janus material during the substitution process. Thanks to angle resolved X-ray photoemission (**AR-XPS**) our analysis is sensitive to the chemical depth profile.



Janus TMDC and Janus Roman god



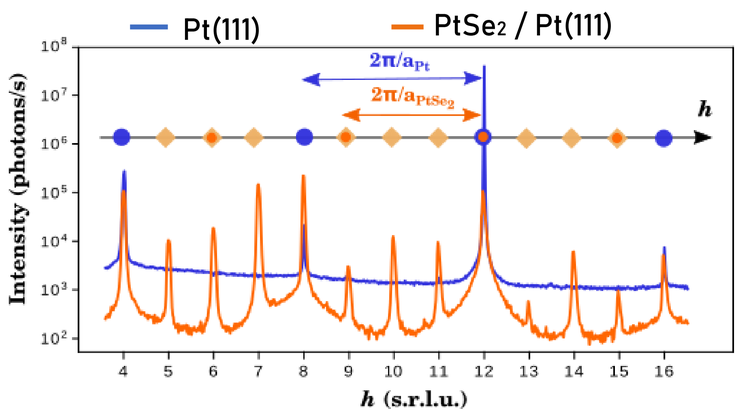
AR-XPS technique schematics

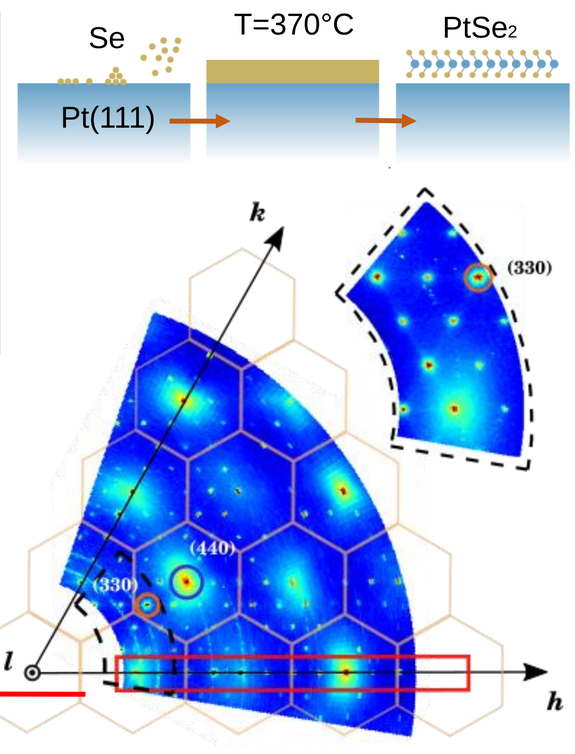

Diffractometer + MBE chamber @BM32

Growth of $PtSe_2$ by selenization of Pt(111)[3]

$PtSe_2$ is grown on Pt(111) by a **two-steps process**[2]:
1) Se deposition on Pt(111)
2) Annealing at 370°C

The as-grown $PtSe_2$ shows a very intense GIXRD pattern with a commensurate **superstructure** due to the exact **3:4** mismatch between Pt(111) and $PtSe_2$ lattice constants.

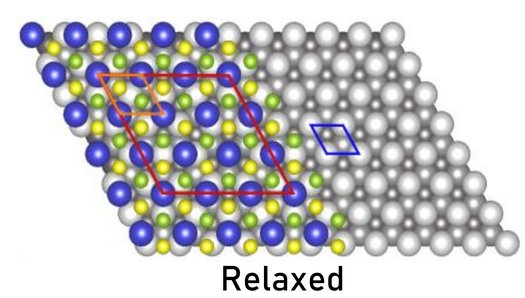


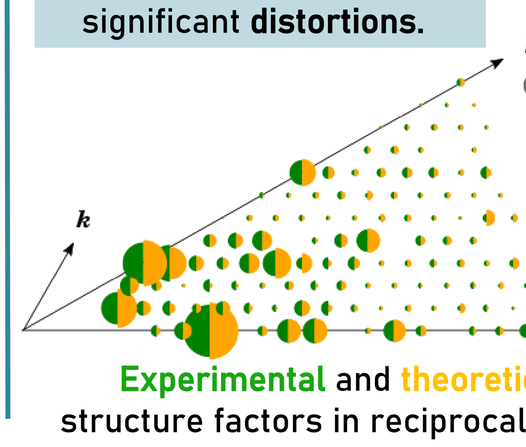


Radial scan and in-plane sector map of the reciprocal space after $PtSe_2$ growth

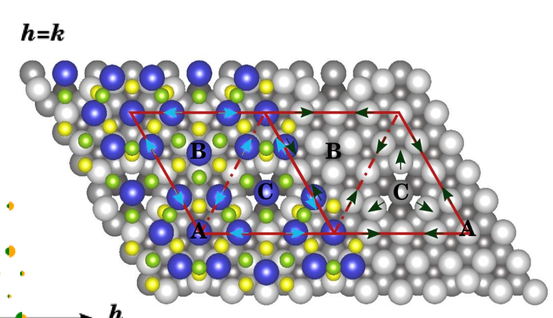
Our **fitting and modelling** of the GIXRD data shows that :

- $PtSe_2$ is **strained** (0.7%)
- The **interface coupling is strong** (not Van der Waals!); both $PtSe_2$ and Pt(111) layers undergo significant **distortions.**


Relaxed



Experimental and theoretical structure factors in reciprocal space



Distorted (fit output)

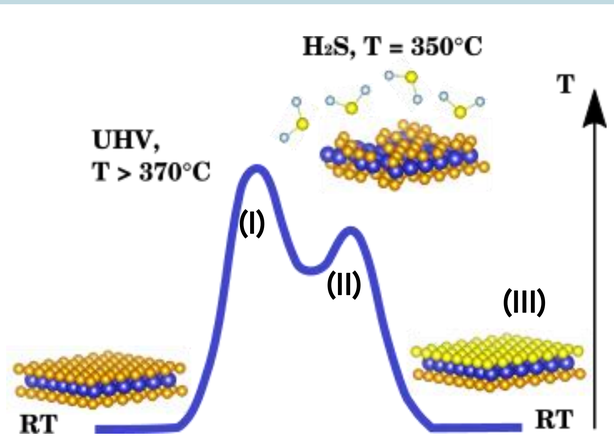
Transformation of $PtSe_2$ into Janus SePtS by sulfurization in H_2S atmosphere[4]

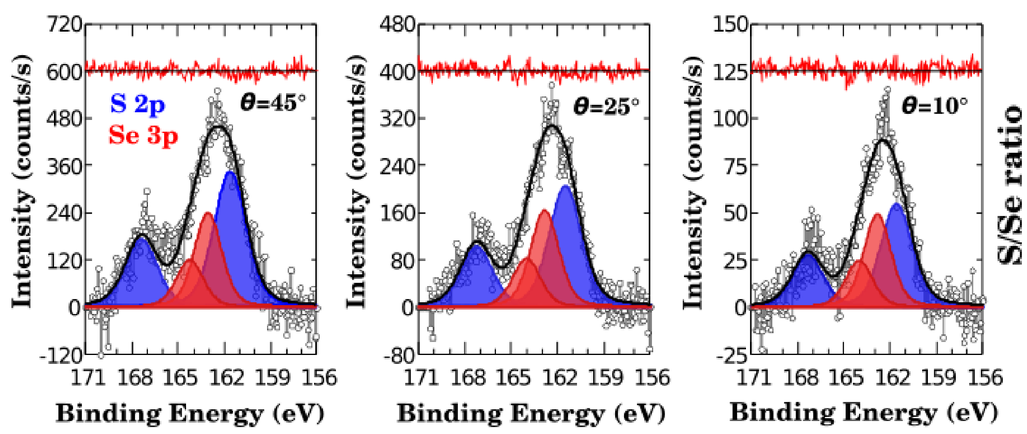
Se in $PtSe_2$ can be replaced by S by supplying **H_2S gas** at a suitable temperature **(sulfurization)** :

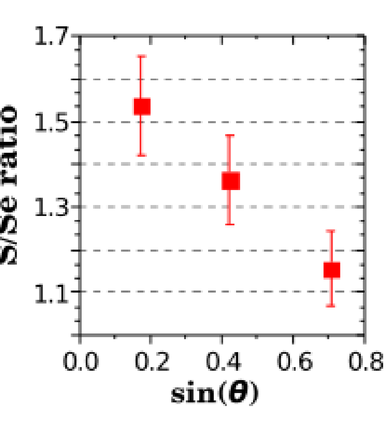
I – a pre-annealing in vacuum creates defects and vacancies in $PtSe_2$.

II –H_2S supplies S to replace Se.

III – Suitable T allows Se-by-S substitution in the top chalcogen layer but not in the bottom one.

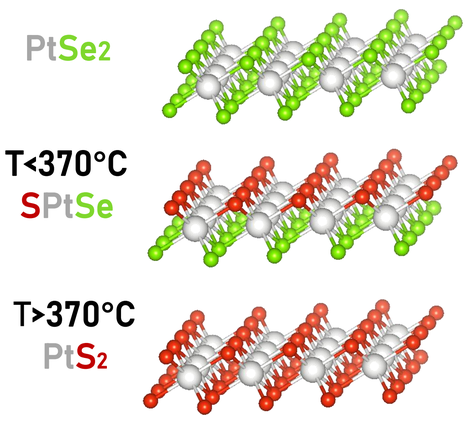


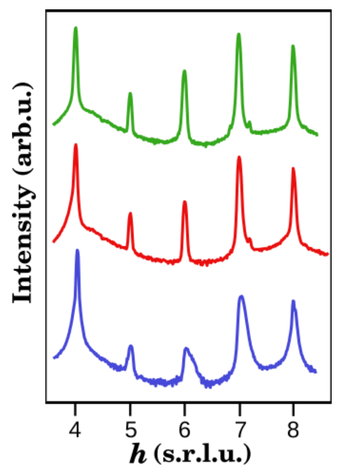


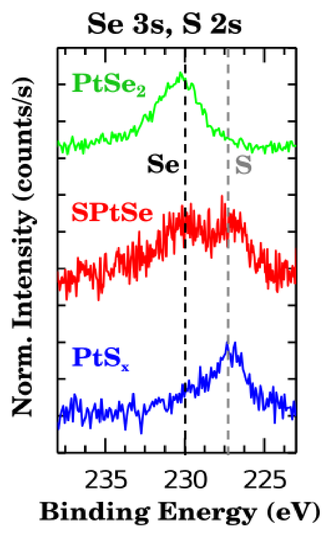


AR-XPS determines that the substitution occurs mostly at the **topmost** surface and S signal comes mostly from **one layer**.

- **Higher T** leads to Se-by-S substitution also in the **bottom** layer.
- The diffraction pattern does not change during the sulfurization. The Janus TMDC is **isostructural** with the pristine $PtSe_2$.







CONTACT PERSON

Roberto Sant
roberto.sant@esrf.fr

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[2] Wang, Y., et al., "Monolayer PtSe2, a new semiconducting transition-metaldichalcogenide …", Nano Lett., 2015.

[3] Sant, R., "Synchrotron x-ray exploration of growth and structure in 2D dichalcogenides" , PhD Thesis, 2019

[4] Sant, R., et al. "Synthesis of epitaxial monolayer Janus SPtSe." , submitted, 2020.

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