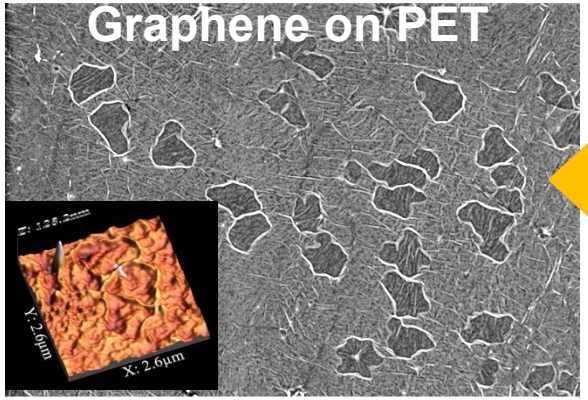
Resolving nanometer-scale variations of doping and strain in single layer MoS_2

Antonis Michail[1], Nikolaos Delikoukos[1], **John Parthenios[1]**, Costas Galiotis[1,3] and Kostantinos Papagelis[1,2]

[1]Foundation of Research and Technology Hellas, Institute of Chemical Engineering Sciences, Patras,Greece
[2]Department of Physics, University of Patras, GR-26504 Patras, Greece
[3]Department of Chemical Engineering, University of Patras, Greece

Native strain and doping in 2D materials

In almost all systems for research and applications 2D materials need to be supported or embedded into other rigid materials including 2D heterostructures

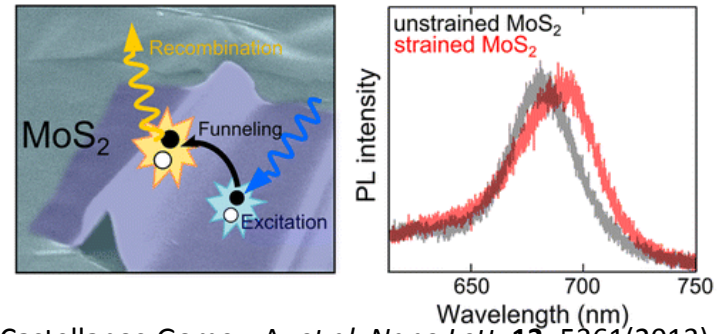


Li *et al*, *ACS-Nano*, 9, 3917-3925, 2015

When supported on solid substrates, van der Waals interactions (interfacial adhesion) induce in- and out-of-plane **structural deformations** and **excess charges.**

Monolayer 2D materials experience uncontrollable mechanical strains via the preparation (e.g., exfoliation or chemical vapor deposition) or the transferring processes

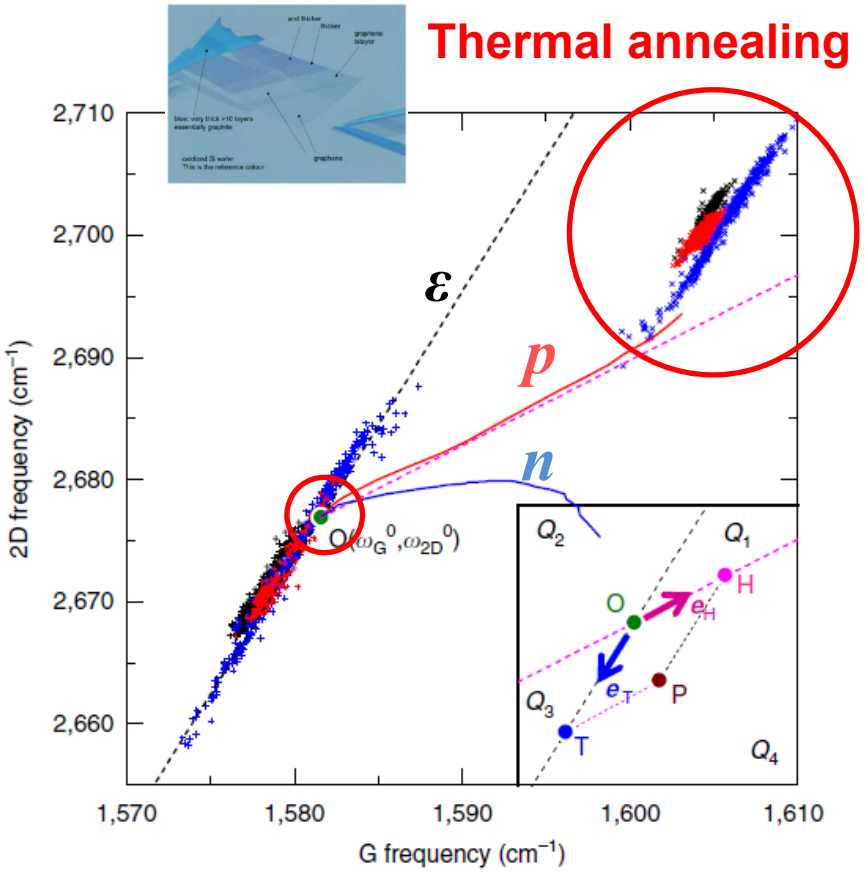
Residual strains and charges can alter significantly the electronic and optical properties of 2D materials (**e.g. band gap in MoS_2**)



Castellanos-Gomez, A. *et al. Nano Lett.* **13,** 5361(2013)

Mechanically exfoliated graphene on SiO_2

It is assumed that graphene strain is biaxial

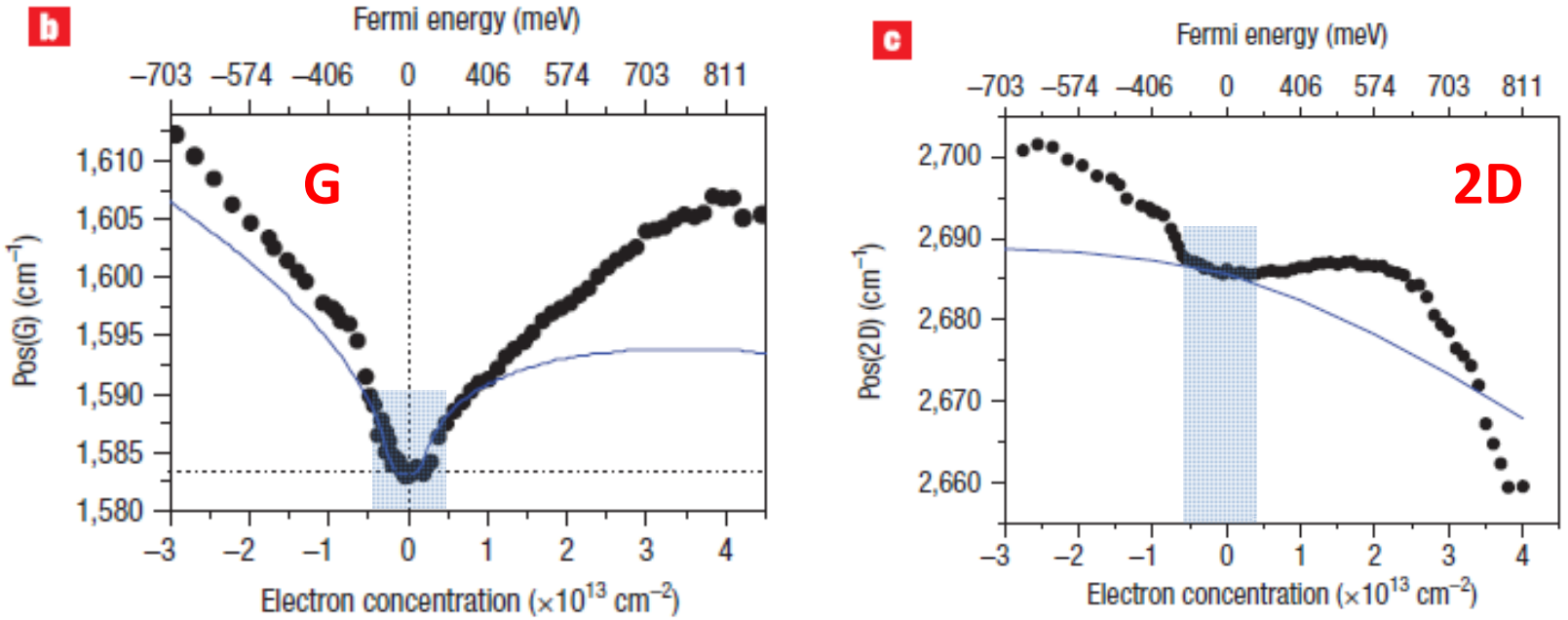


Vector decomposition of **strain (ε)** & **charge density (*p* or *n*)**

Pos(2D) vs Pos(G) slope ~ 2.3 - 2.5 (strain dominated)

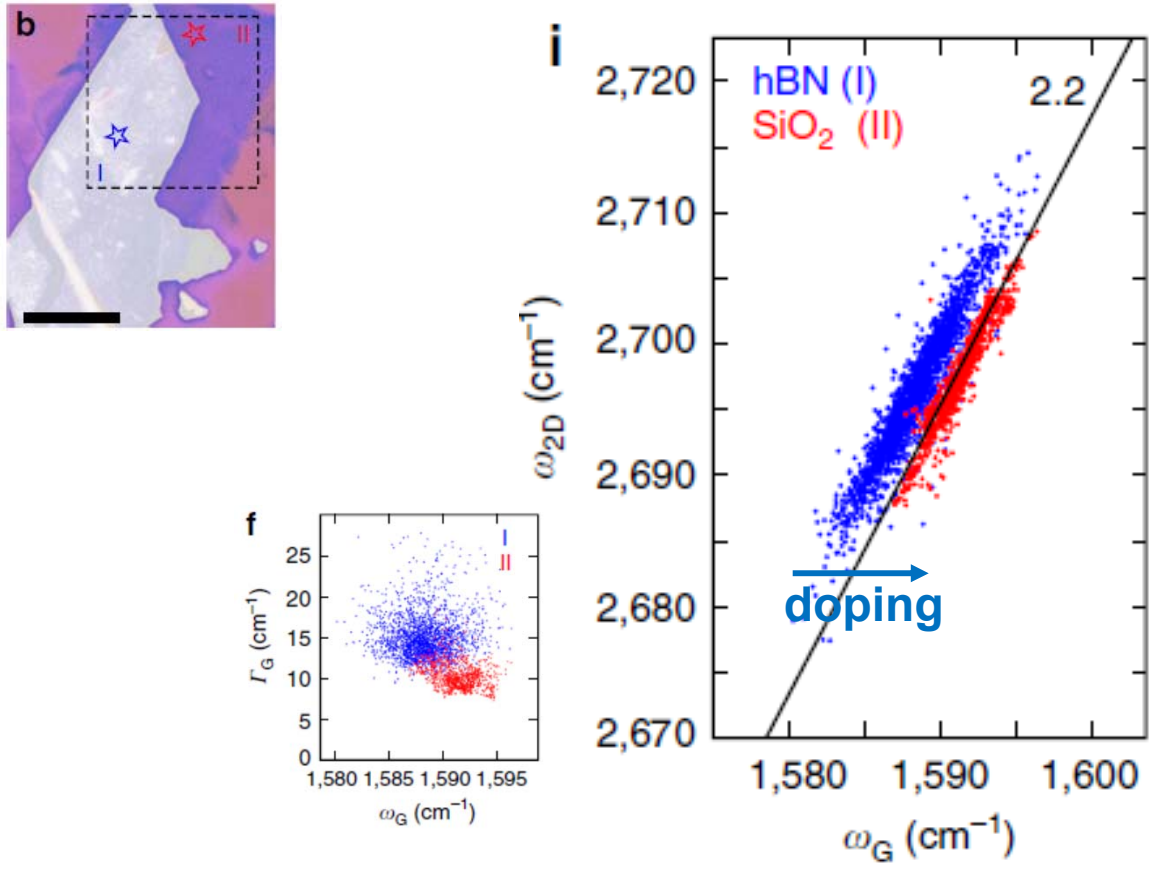
* Lee, J. E., *et al*. *Nat Commun* **3,**1024 (2012).

G & 2D *vs* doping in exfoliated graphene on SiO_2



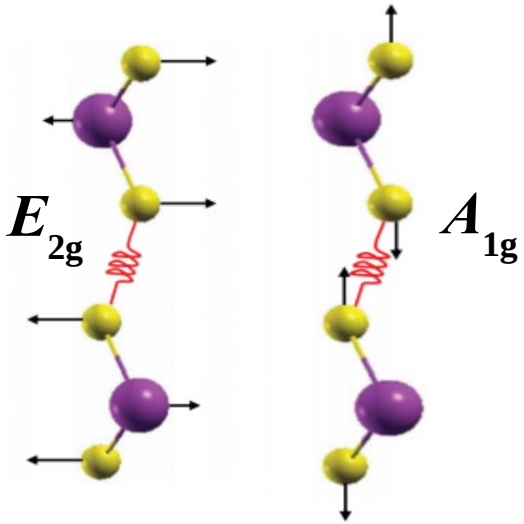
Das, A. *et al.* *Nature Nanotechnology* **3,** 210(2008)

Mechanically exfoliated graphene on *h* – BN on SiO_2

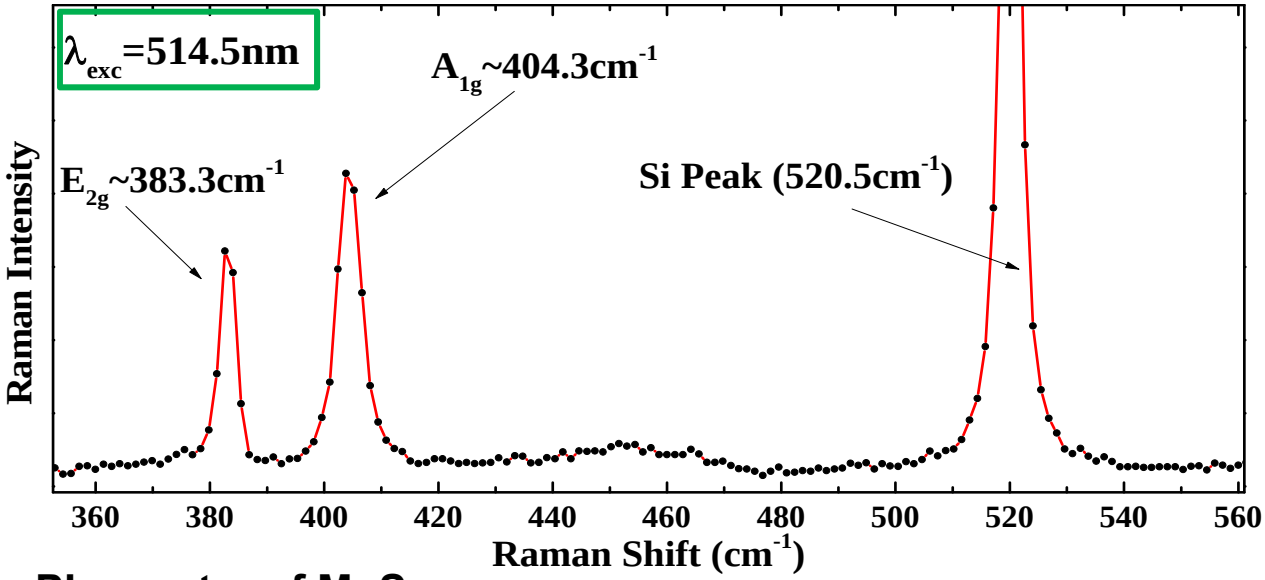


* C. Neuman., *et al*. *Nat Commun* **6,**8429 (2015).

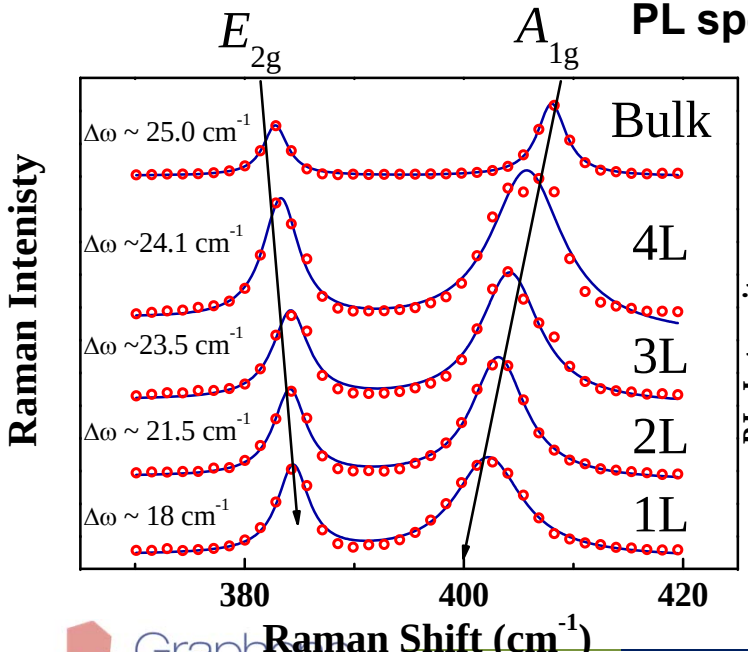
Raman & PL spectroscopy of few layer MoS_2

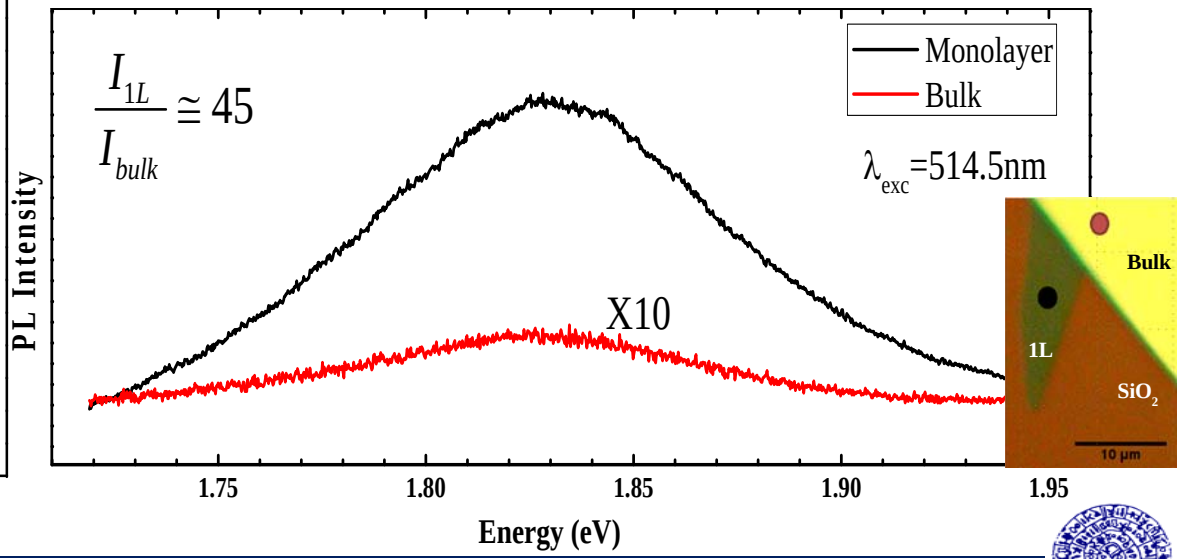


Phys. Rev. B **84**, 155413



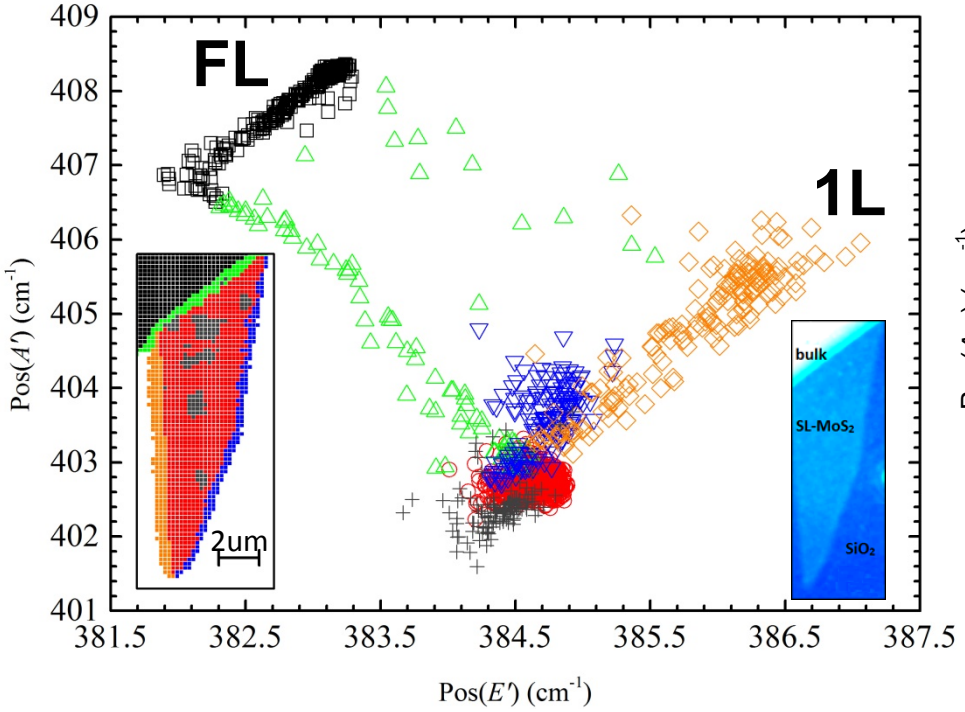
PL spectra of MoS_2



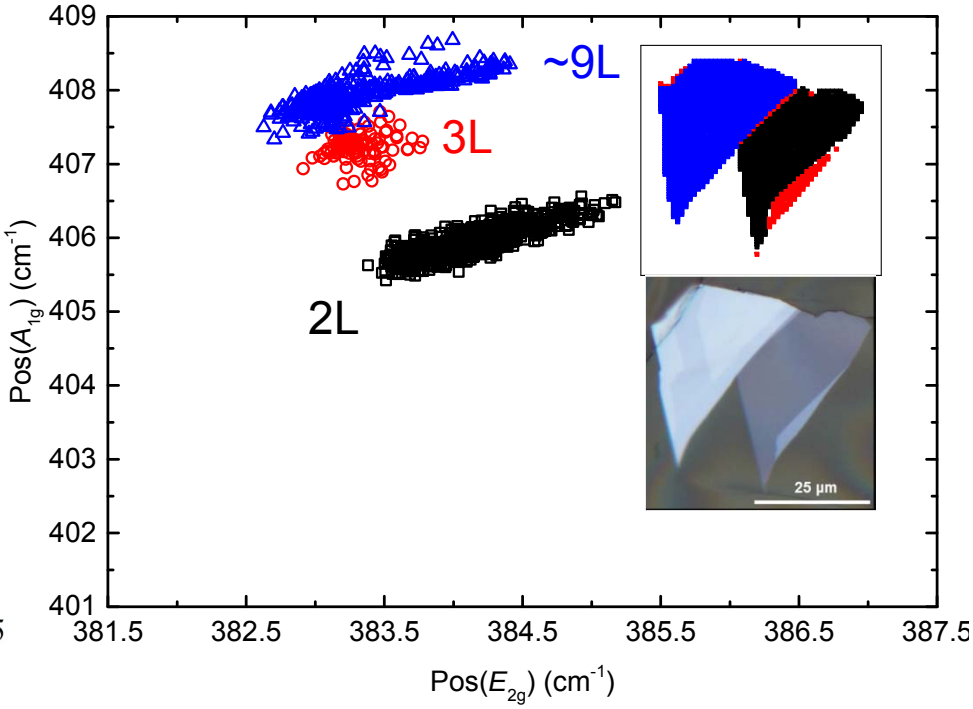


Pos(A_{1g}) *vs* Pos(E_{2g}) of MoS_2 flakes on different substrates

On SiO_2



On PMMA



- λ_{ecx} = 514.5 nm
- Scanning step = 0.2 μm
- 25 spectra/ μm^2 or **3000** spectra

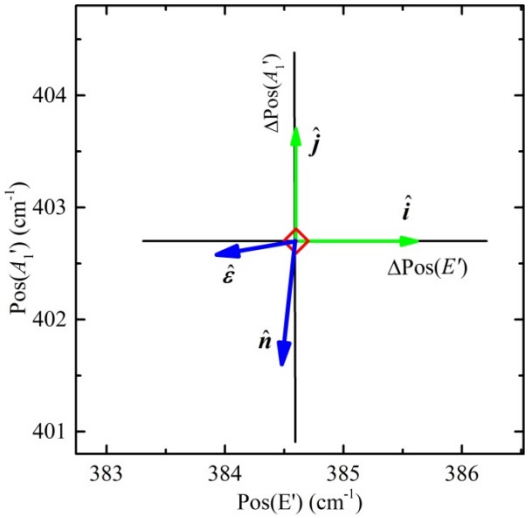
$(\hat{\varepsilon},\hat{n})$ space determination

$$\delta\omega_{tot} = \delta\omega_{strain} + \delta\omega_{doping}$$

$$\delta\omega_{strain} = -2\gamma\omega_o\varepsilon_{biaxial} \qquad \gamma = -\frac{1}{\omega_o}\frac{\partial\omega}{\partial\varepsilon_h}$$

$$\delta\omega_{doping} = -k_n n \quad k_n = \frac{\partial\omega}{\partial n}$$

$$\begin{pmatrix} \Delta\mathrm{Pos}(E') \\ \Delta\mathrm{Pos}(A_1') \end{pmatrix} = \begin{pmatrix} -2\gamma(E')\mathrm{Pos}(E')_0 & k_n(E') \\ -2\gamma(A_1')\mathrm{Pos}(A_1')_0 & k_n(A_1') \end{pmatrix} \begin{pmatrix} \varepsilon \\ n \end{pmatrix}$$

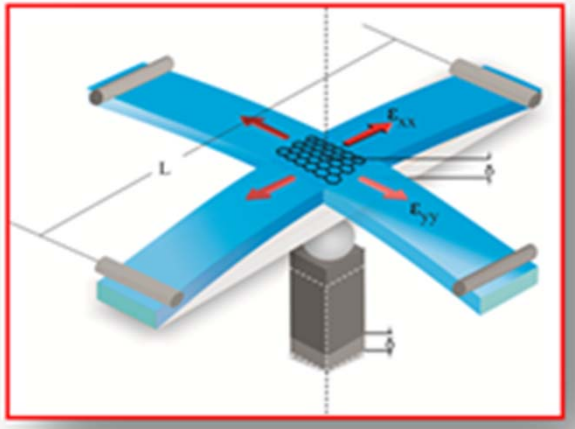


	γ	k_n (×10^{-13} cm)
E’	1.08 (exp)	-0.33
A_1'	0.15	-2.22

Chakraborty B. Physical Review B, 2013. **87**(8)

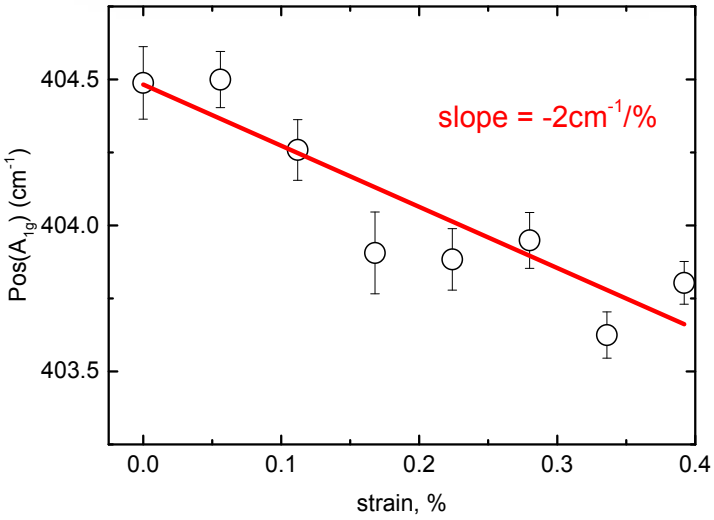
Biaxial deformation of single layer MoS_2

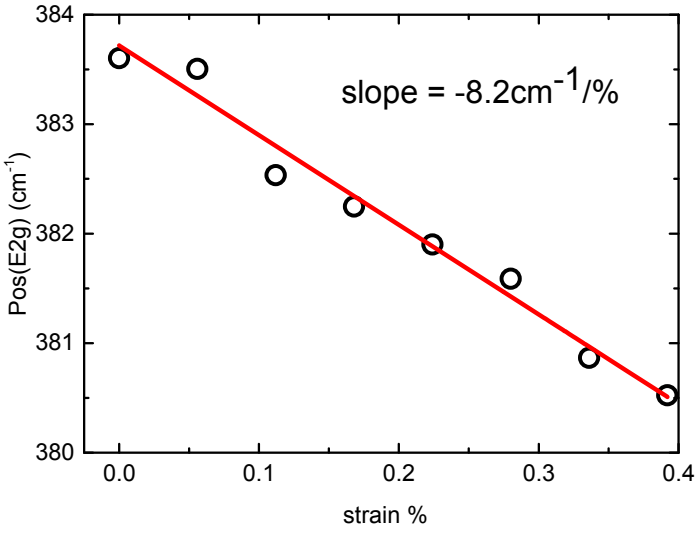
Measuring the Gruneisen parameter



Androulidakis C. et al., Sci. Rep. 5, 18219 (2015)

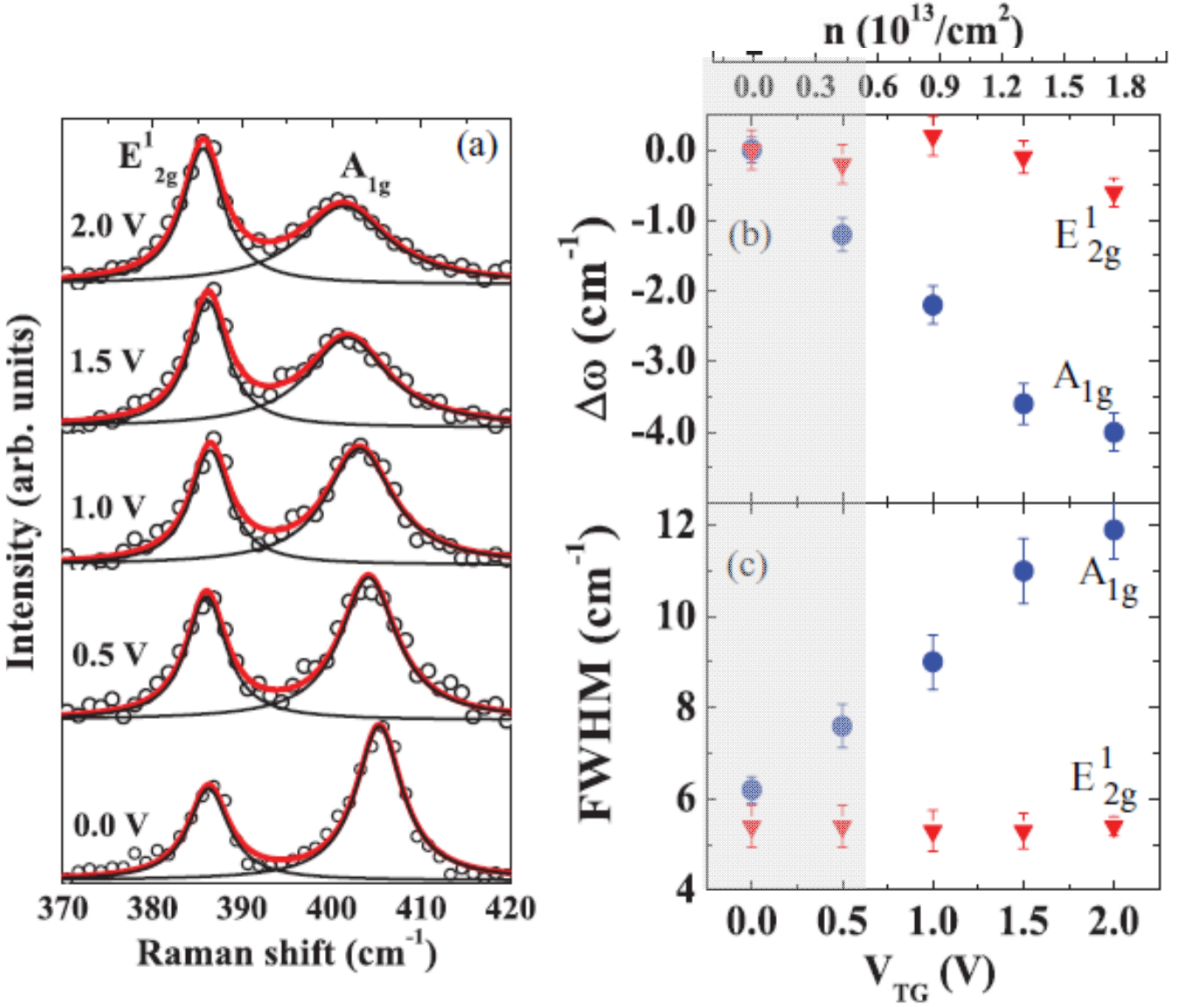
$$\gamma(\omega) = -\frac{1}{\omega_0}\frac{\delta\omega_{strain}}{2\varepsilon_{biaxial}}$$





Unpublished data

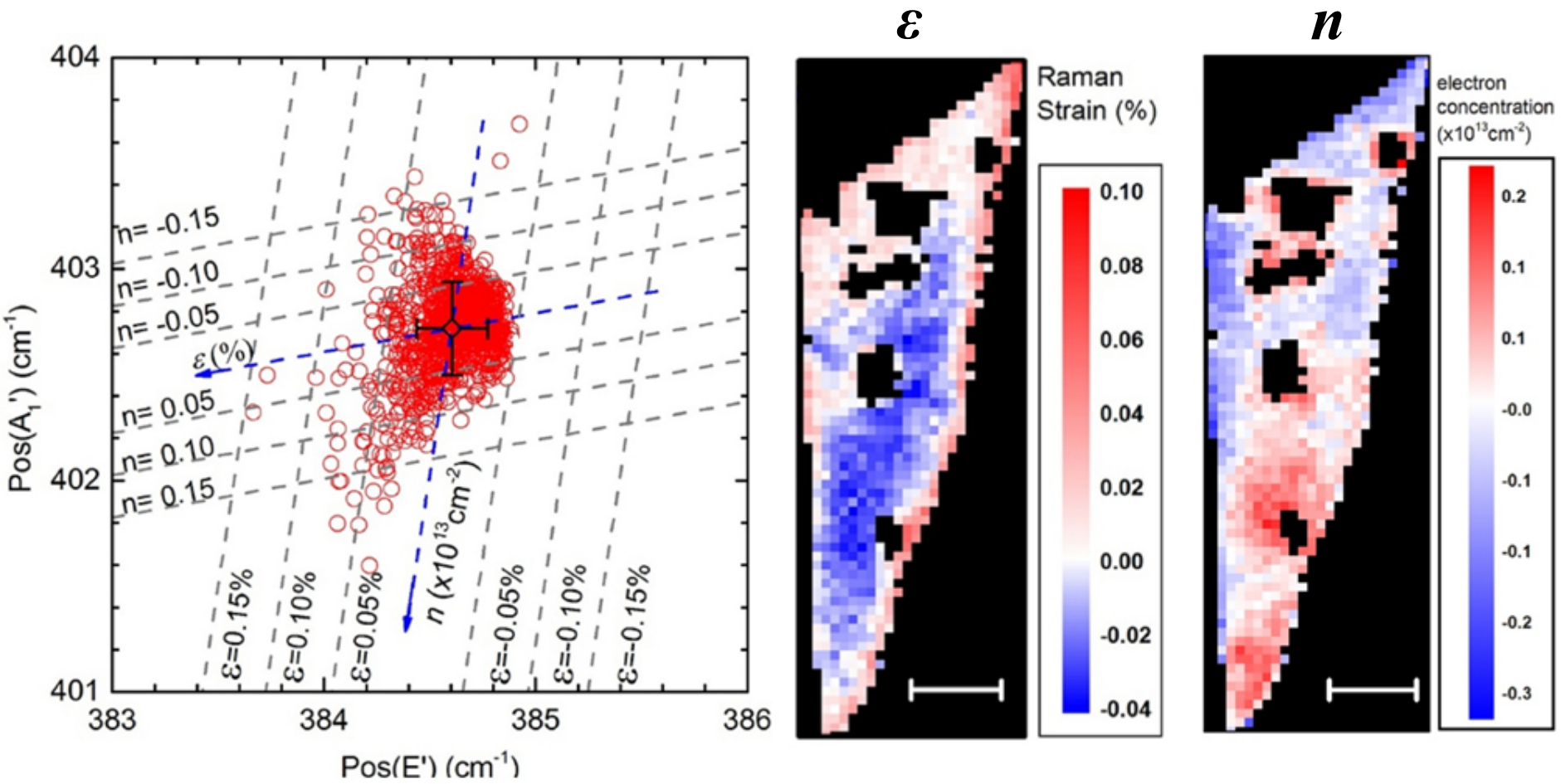
The effect of doping in 1L exfoliated MoS_2 on SiO_2



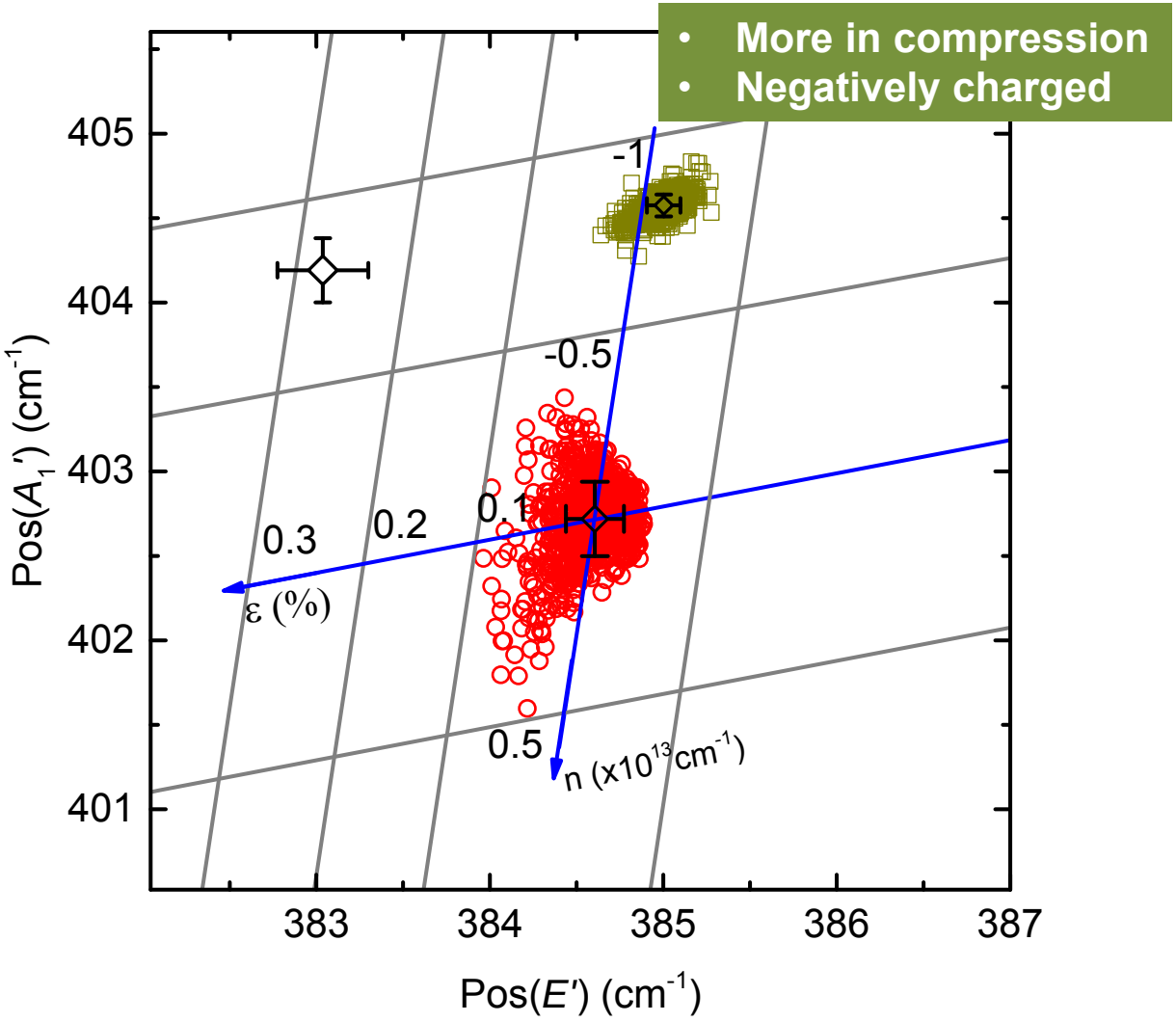
E_{1g} is less sensitive in doping than A_{1g}

Chakraborty, B. et al. Phys. Rev. B 85, 161403 (2012)

Pos(A_1') vs Pos(E') and the $(\hat{\varepsilon},\hat{n})$ space

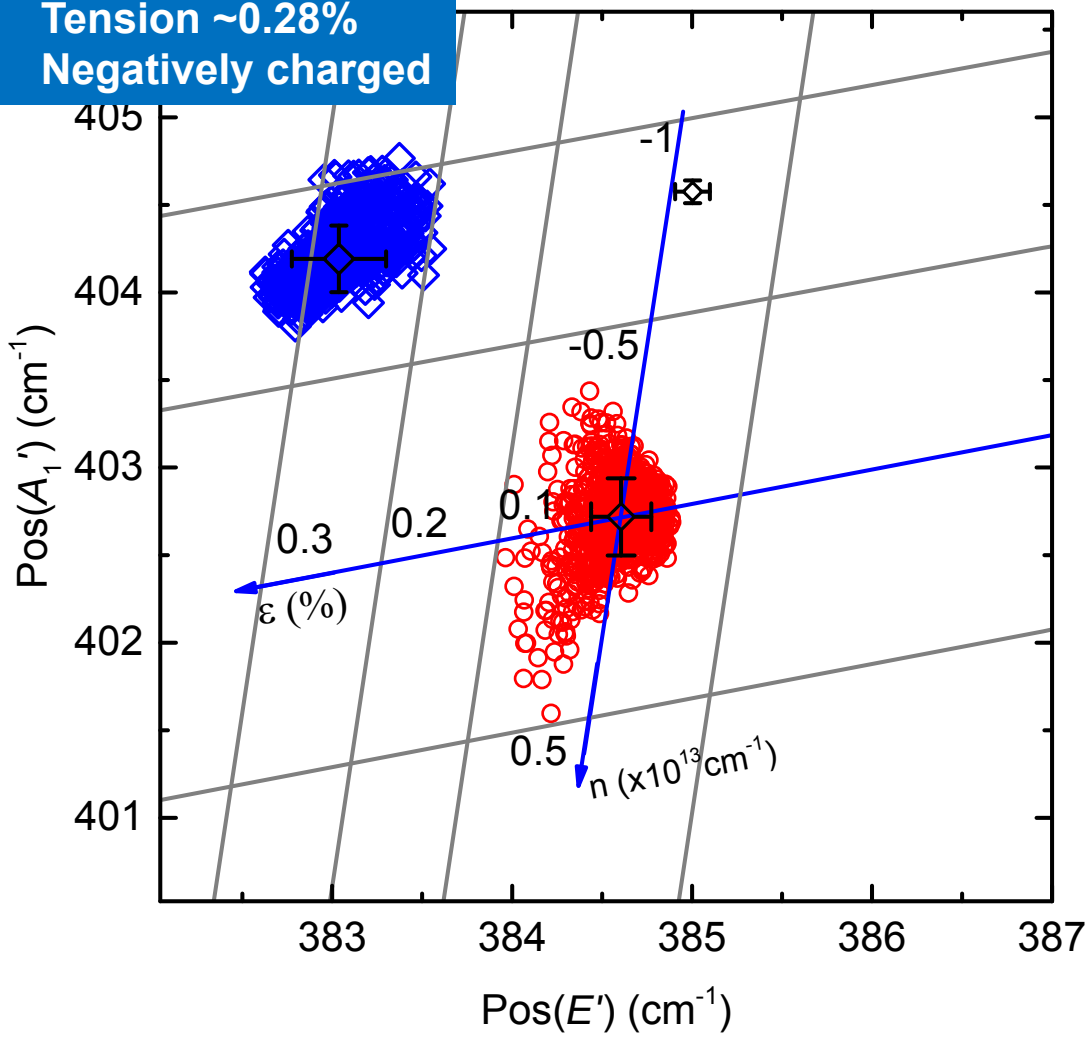


Pos(A') *vs* Pos(E')
1L MoS_2 exfoliated onto SiO_2

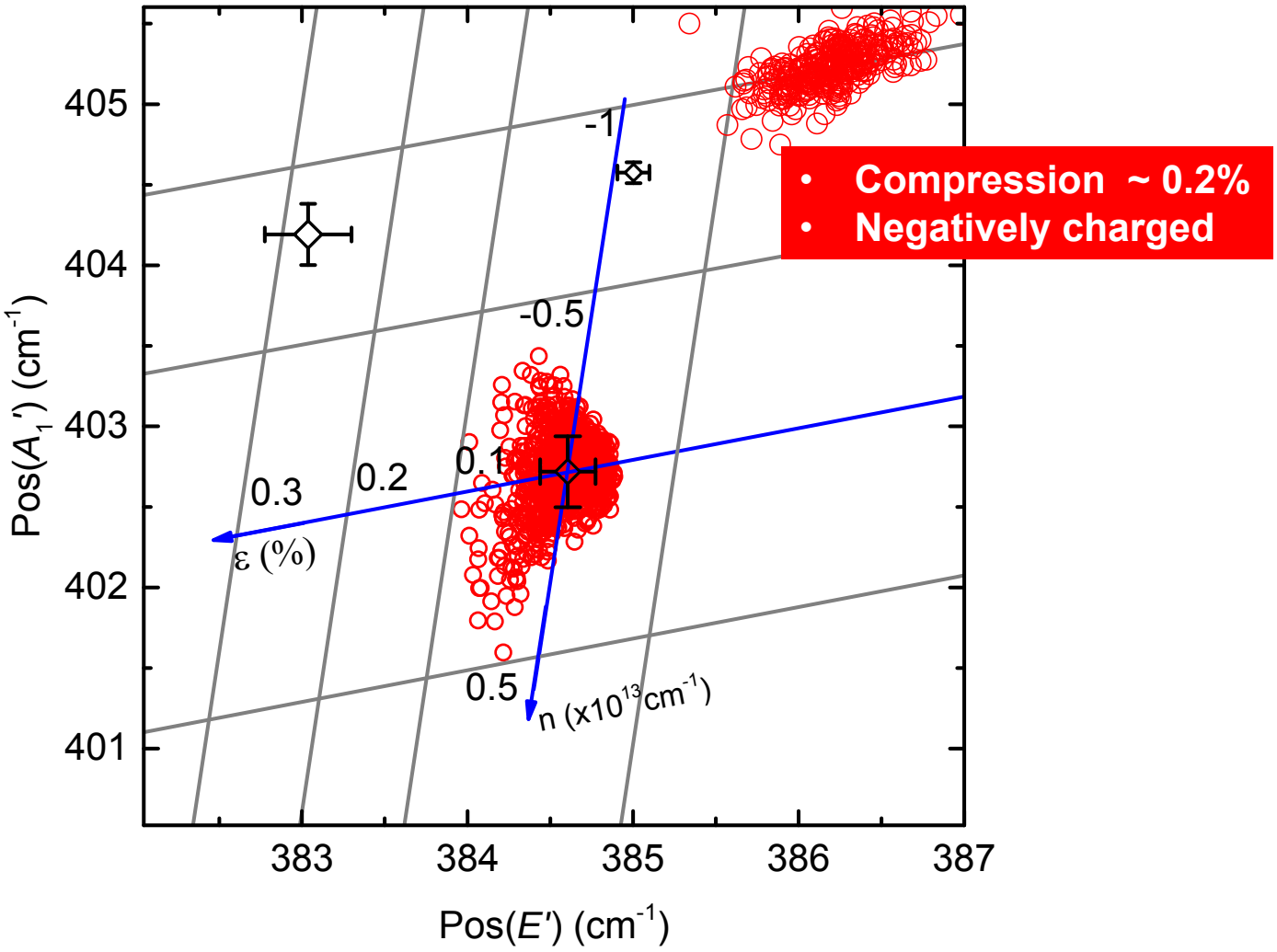


Pos(A') *vs* Pos(E')
1L MoS_2 grown onto SiO_2 by CVD

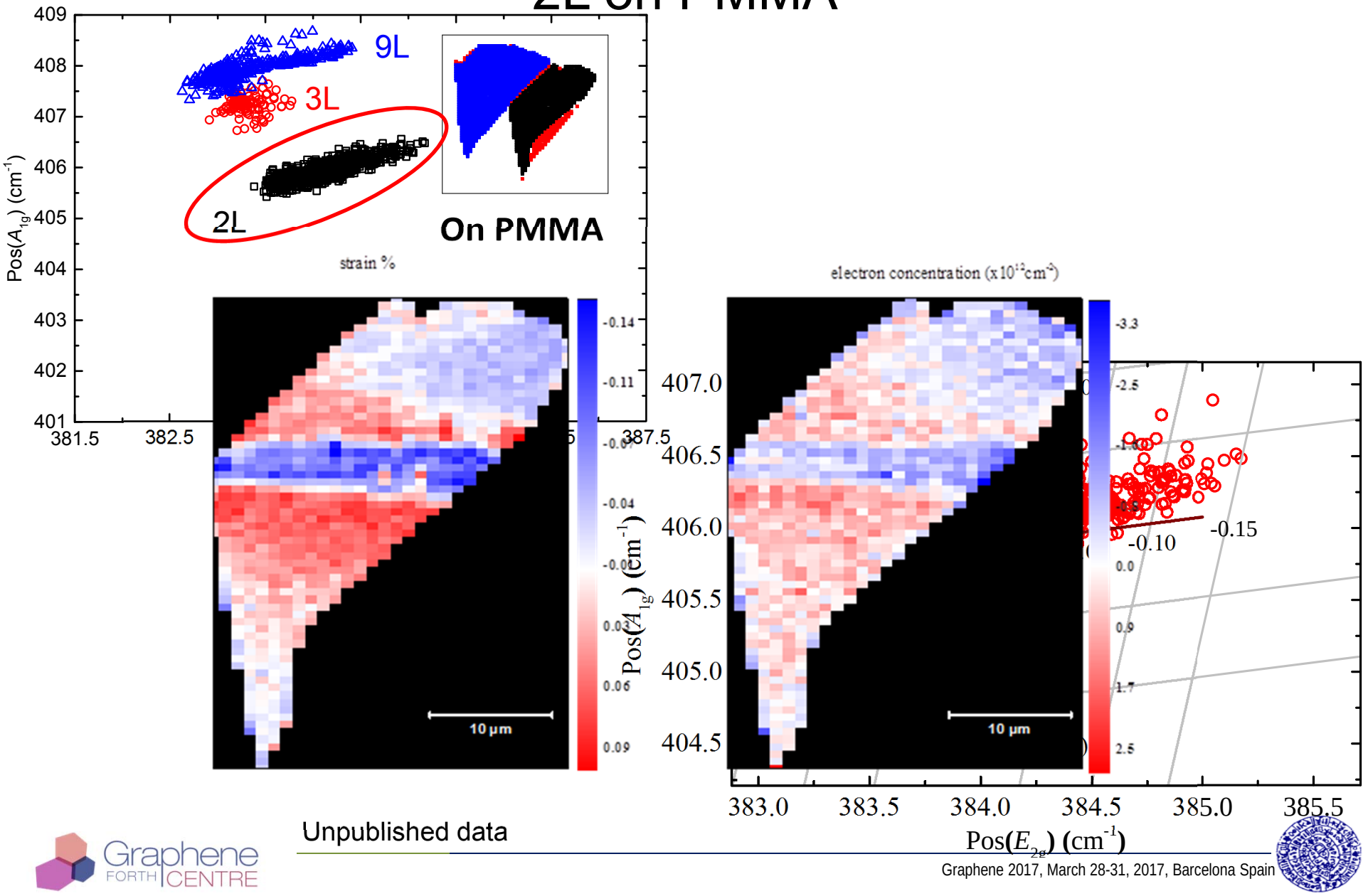
- Tension ~0.28%
- Negatively charged



Pos(A') *vs* Pos(E')
CVD grown 1L MoS_2 transferred onto PMMA



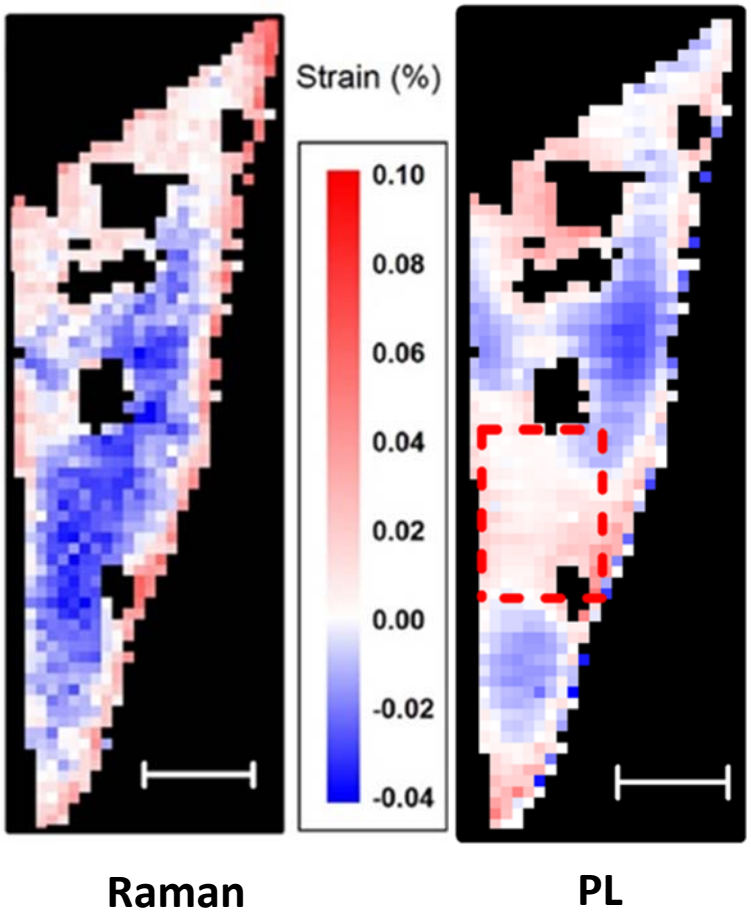
Pos(A_1') vs Pos(E') and the $(\hat{\varepsilon},\hat{n})$ space
2L on PMMA

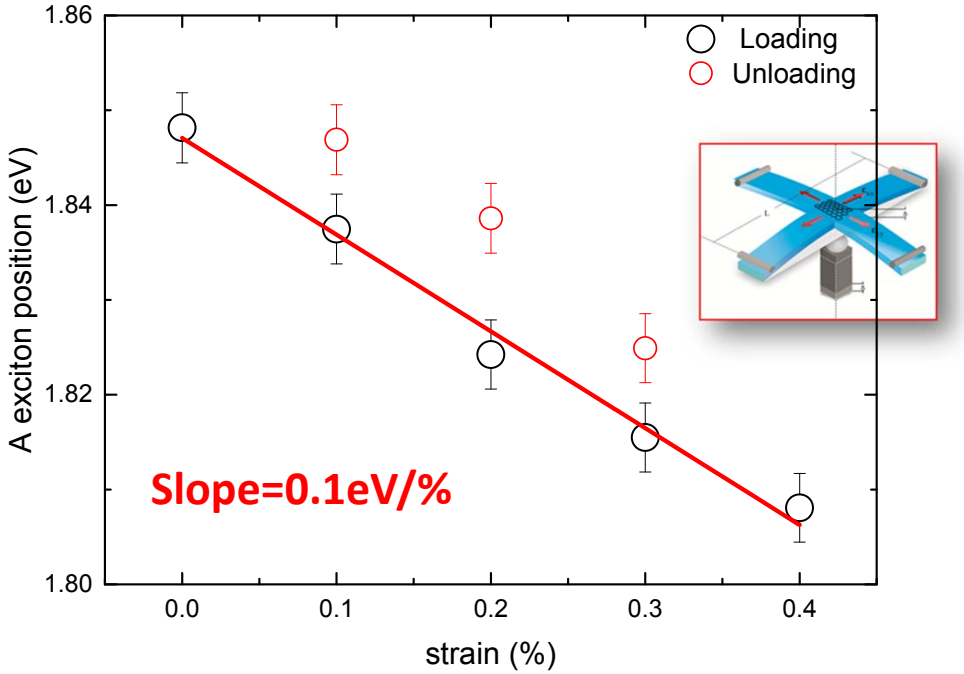


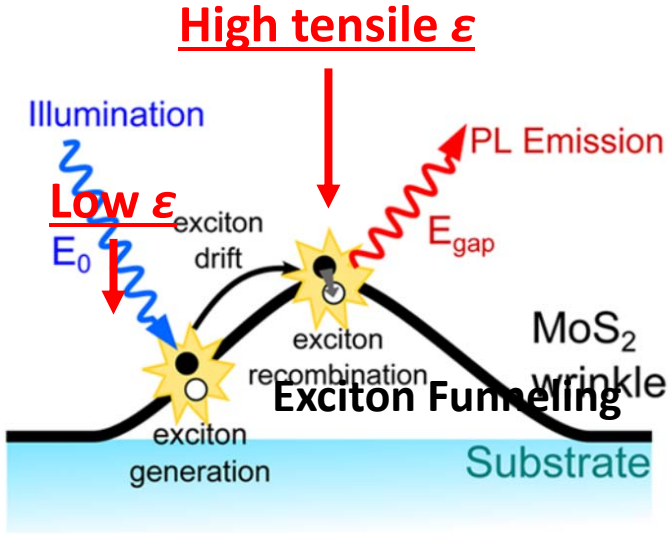
Unpublished data

Strain evaluation using PL

$$\Delta E_g = (-0.1eV/\%)\varepsilon_{biaxial}$$



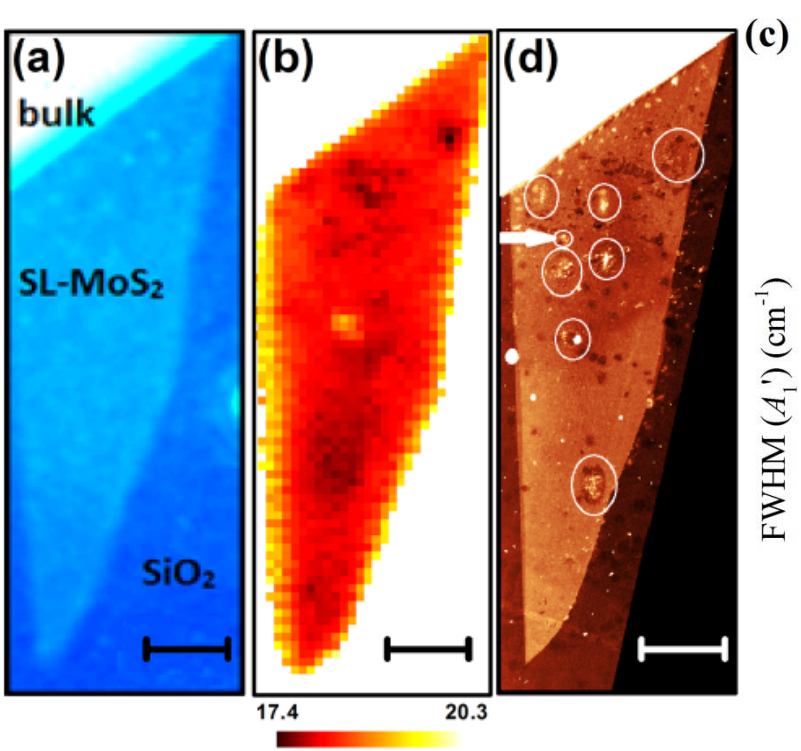




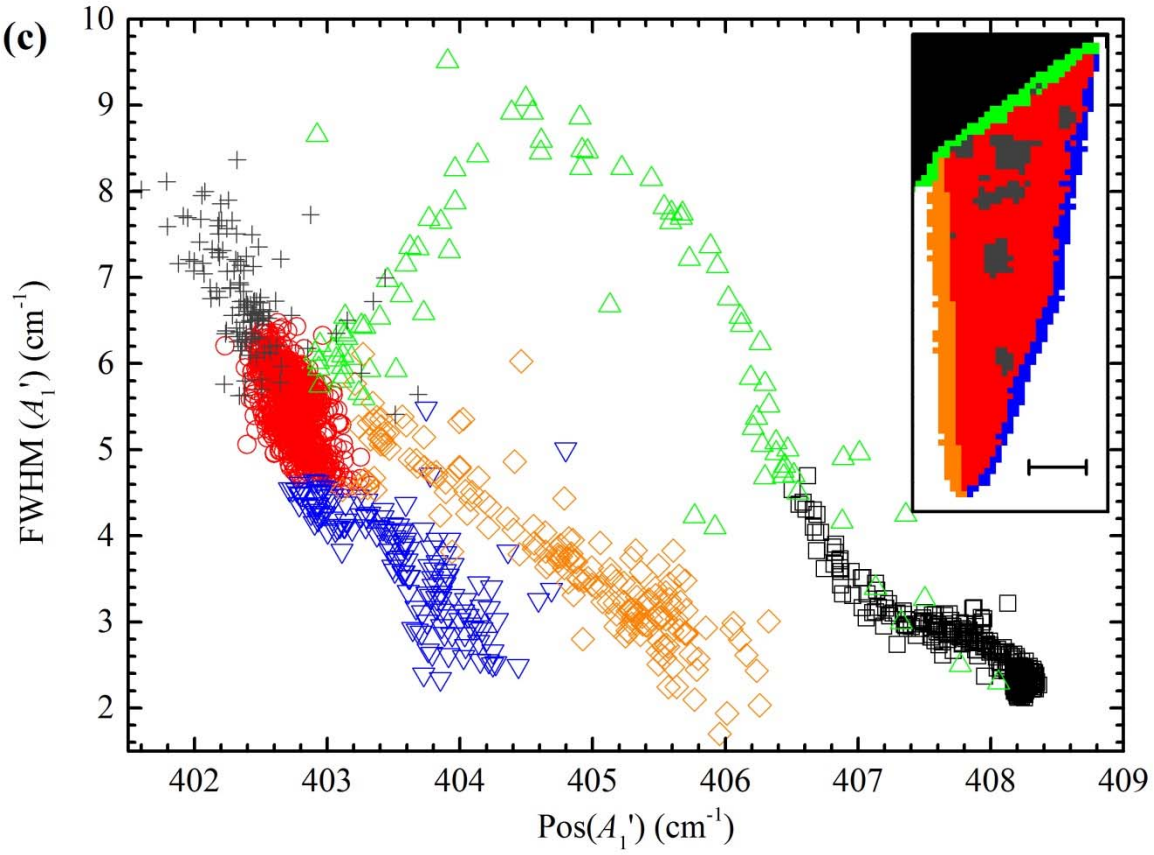
Michail et al. Applied Physics Letters, 2016. **108**(17): p. 173102

Nano Letters, 2013. **13**(11): p. 5361-5366

FWHM(A_1') *vs* Pos(A_1')



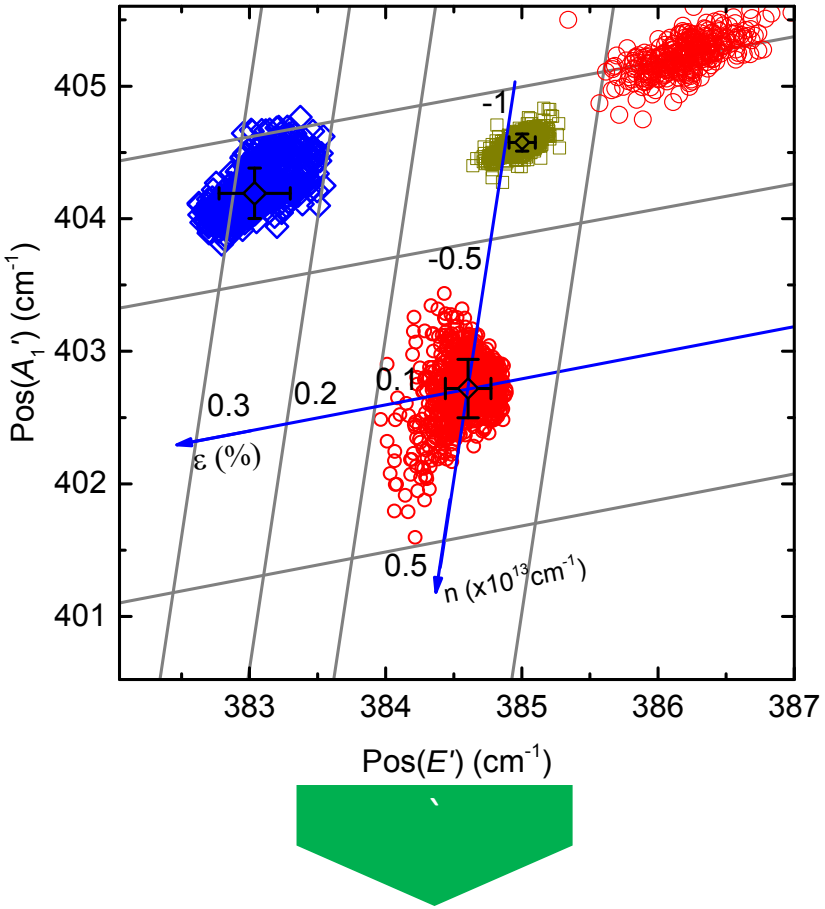
Scale bar: **2μm**



- Discriminate defects with spatial resolution below 1 μm
- Voight profiles to deconvolute the spectrograph response

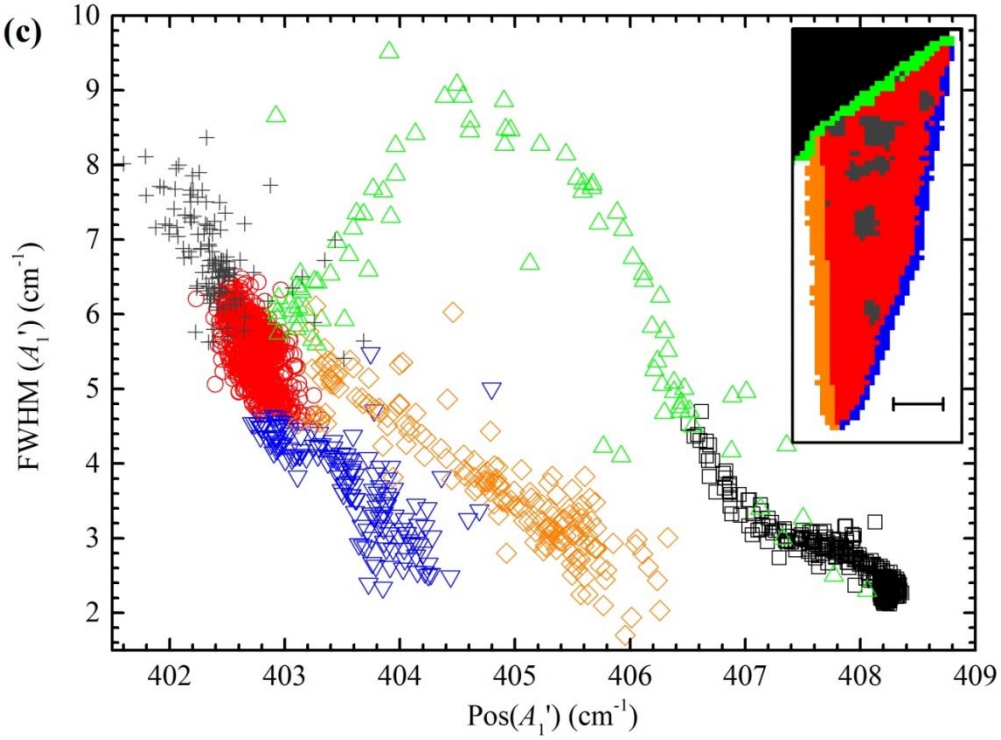
Conclusions

Correlation I



ε, *n* deconvolution

Correlation II



Discrimination of structural features with spatial resolution below 1 μm

ACKNOWLEDGEMENTS

GRAPHENE FLAGSHIP

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Thanks very much for your attention