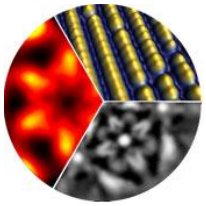
UNIVERSITÉ DE FRIBOURG
UNIVERSITÄT FREIBURG

Electron Spectroscopy Group



A local real-space view of the periodic lattice distortion in 1*T*-$TiSe_2$

A scanning tunneling microscopy and DFT study

B. Hildebrand, T. Jaouen, M-L. Mottas, G. Monney, and P. Aebi — *University of Fribourg*

DFT calculations :
D. R. Bowler — *London Centre for Nanotechnology*

Growth of Single Crystals :
C. Barreteau, E. Giannini — *University of Geneva*

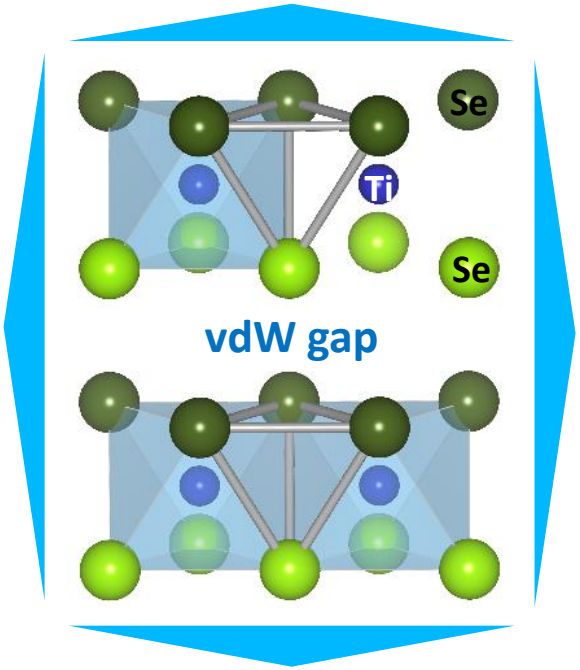
⟨S|P|S⟩ swiss physical society

FNSNF Fonds national suisse Schweizerischer Nationalfonds Fondo nazionale svizzero Swiss National Science Foundation

frimat

Motivation

1*T*-$TiSe_2$: an intriguing compound



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Cu doped 1*T*-$TiSe_2$

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Under pressure

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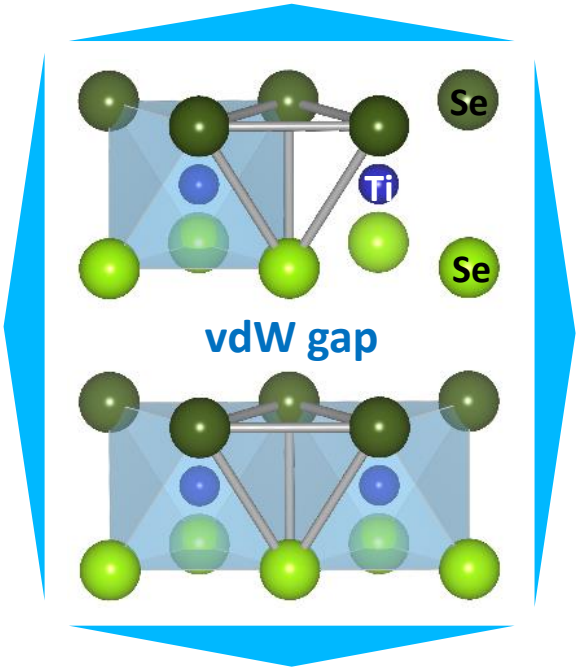

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T_{CDW} ~ 200 K, new 2x2x2 structure

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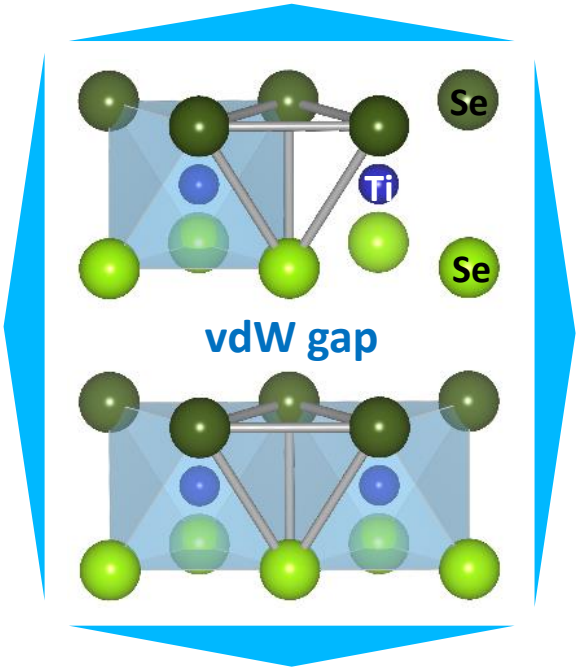

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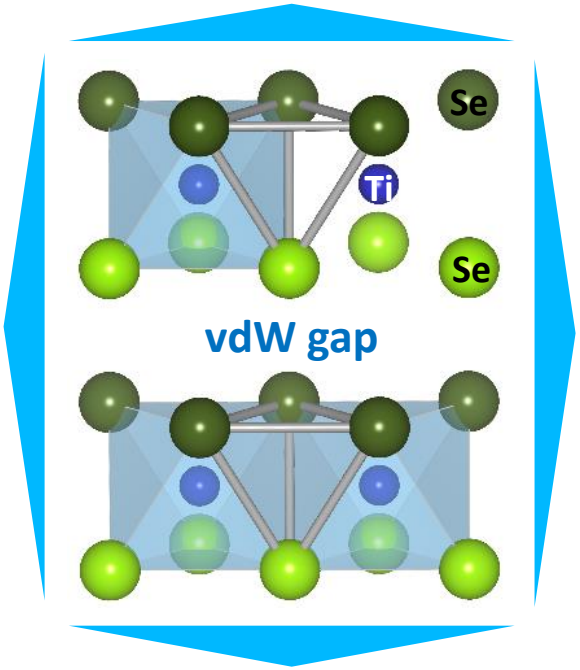
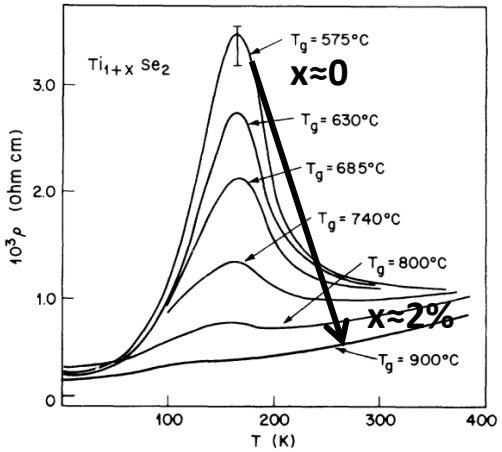


Anomalous resistivity



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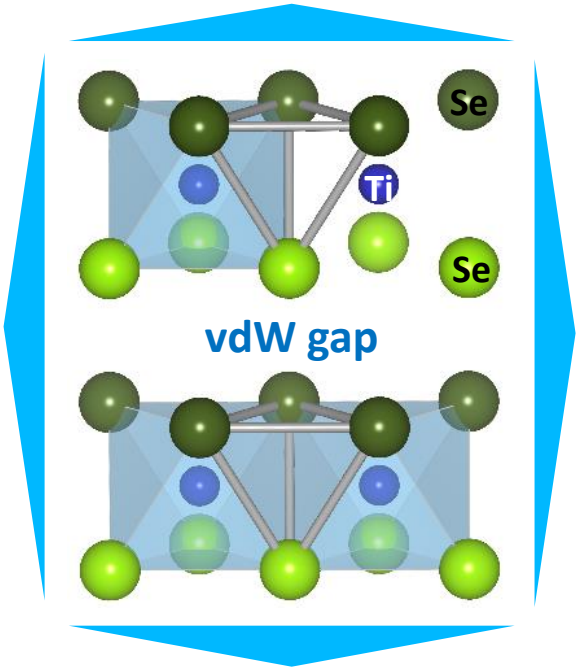

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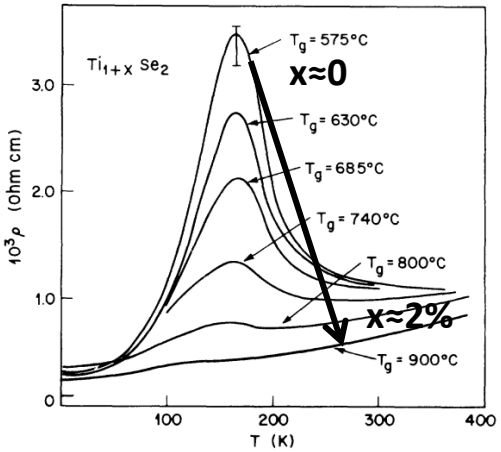

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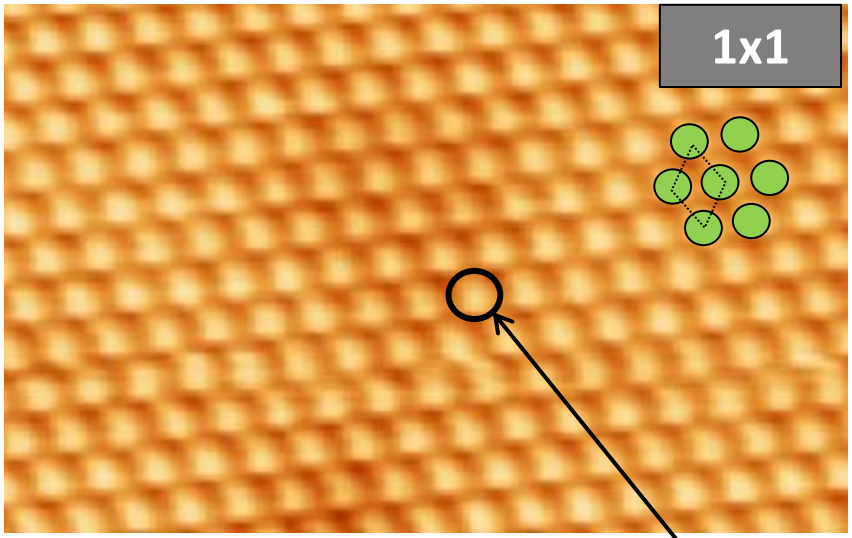
What is the signature of the CDW/PLD with STM ?

The 1*T*-$TiSe_2$ CDW viewed by STM



V_{bias}=-1 V

The topmost layer of 1*T*-$TiSe_2$ is a Se layer.

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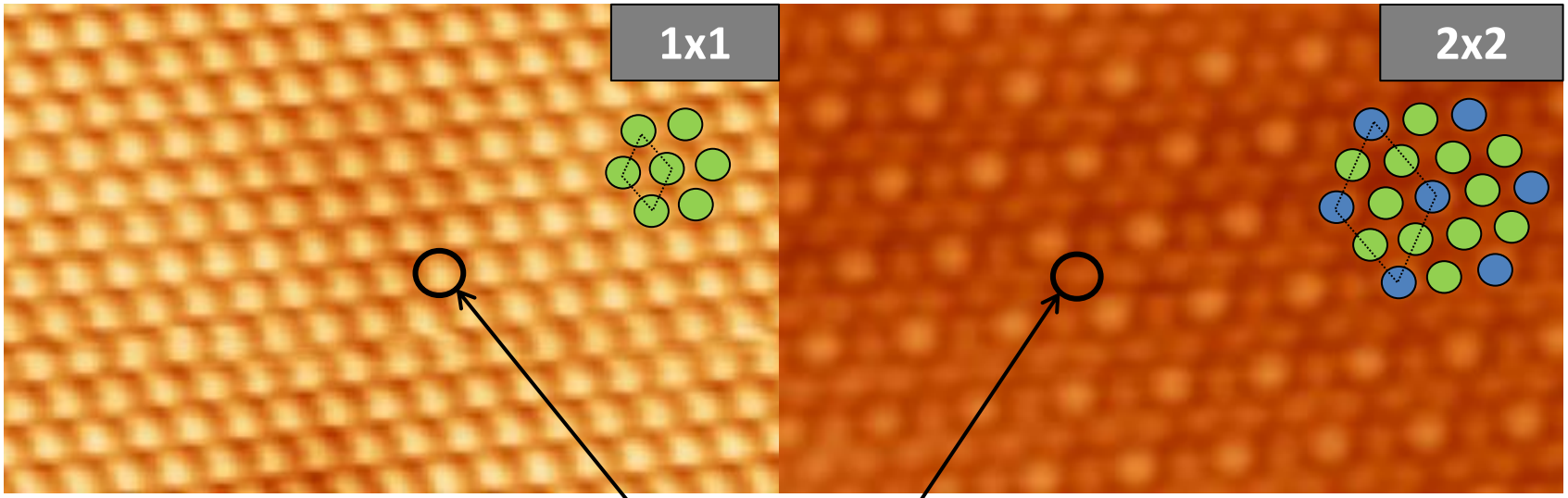

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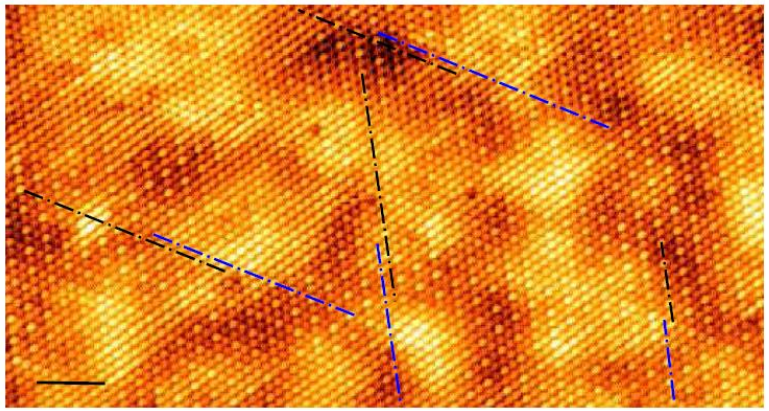
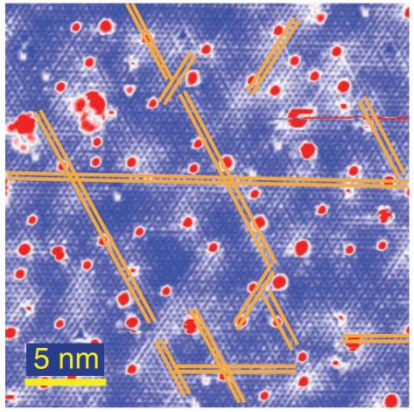
Domains and chirality observed with STM

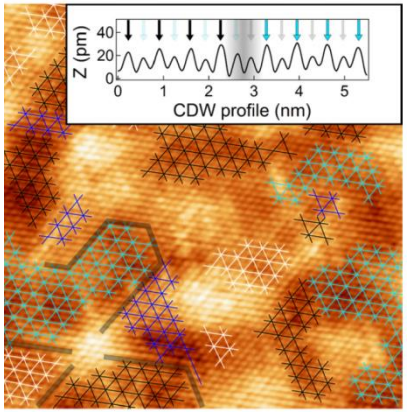
Domain formation upon doping (Cu or Ti)



A. M. Novello, PRL, **118**, 017002 (2017)



S. Yan, PRL, **118**, 106405 (2017)



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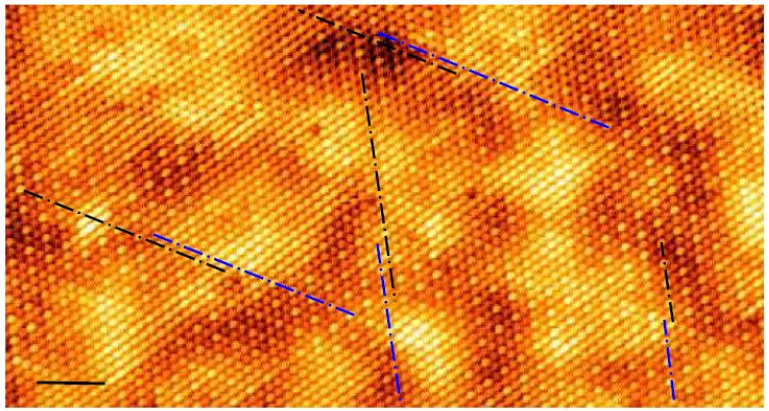

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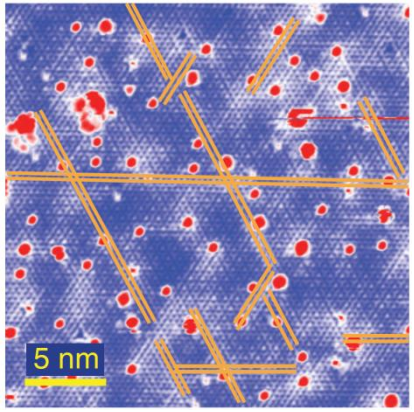

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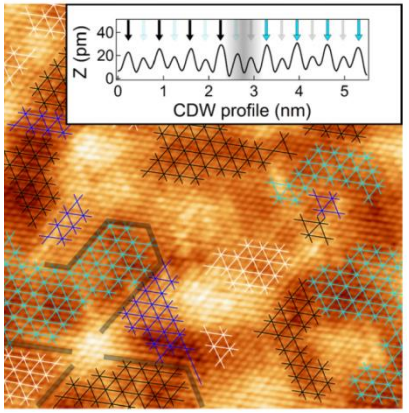

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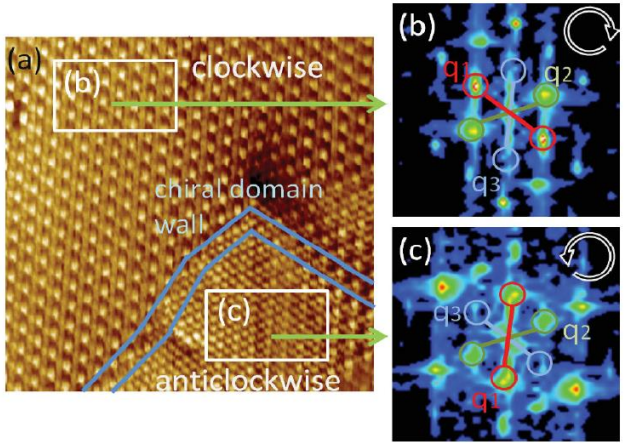
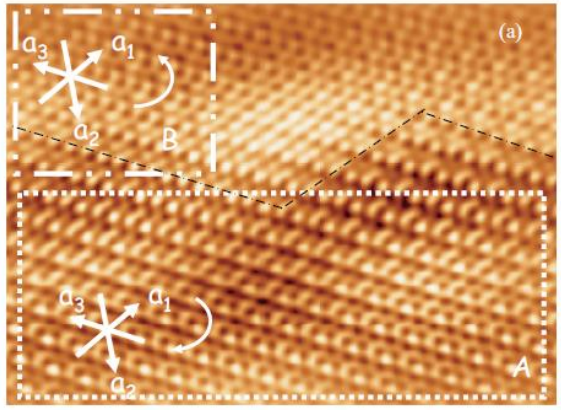
Chiral CDW

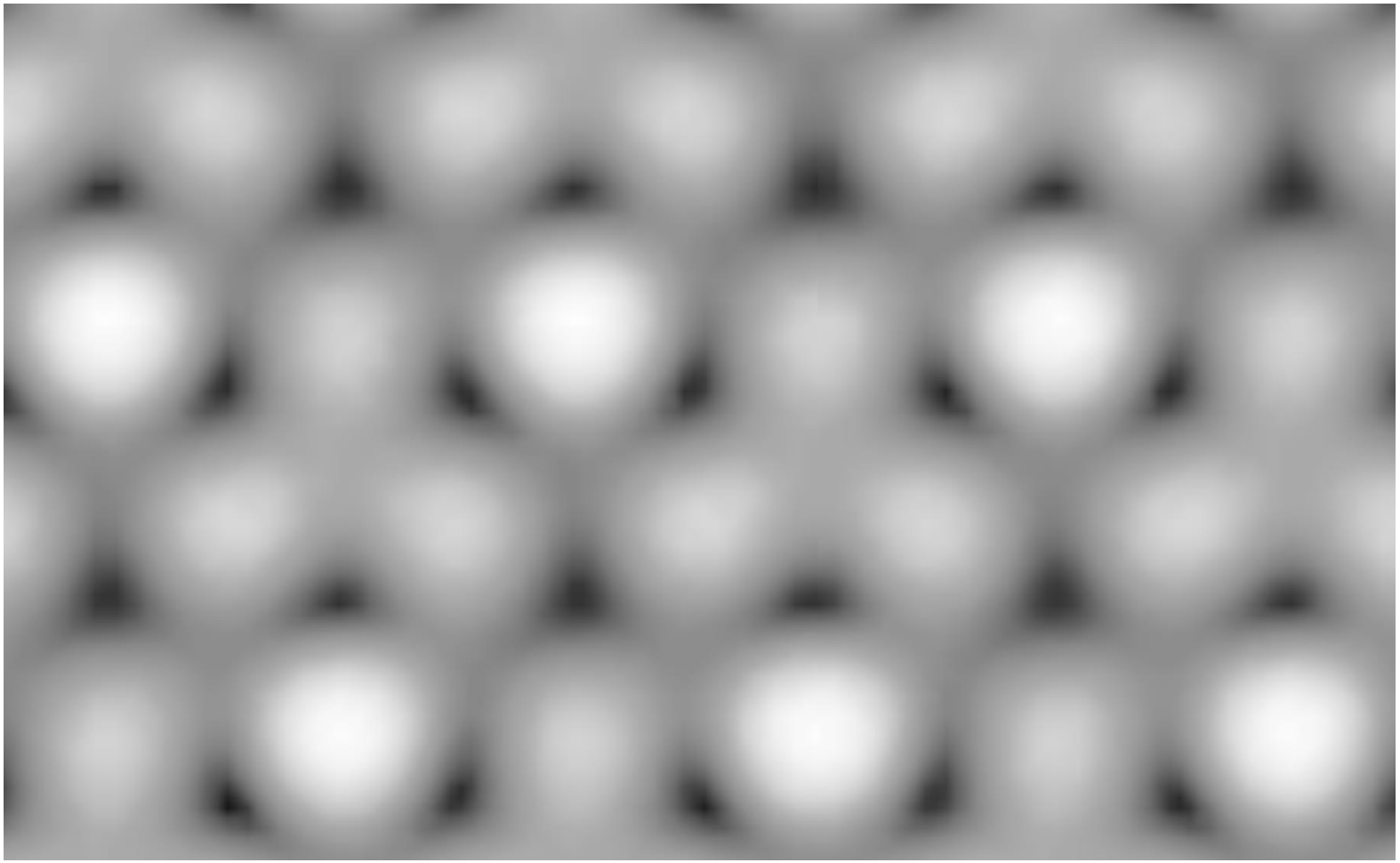


J. Ishioka, PRL **105**, 176401 (2010)



M. Iavarone, PRB **85**, 155103 (2012)

The importance of the PLD



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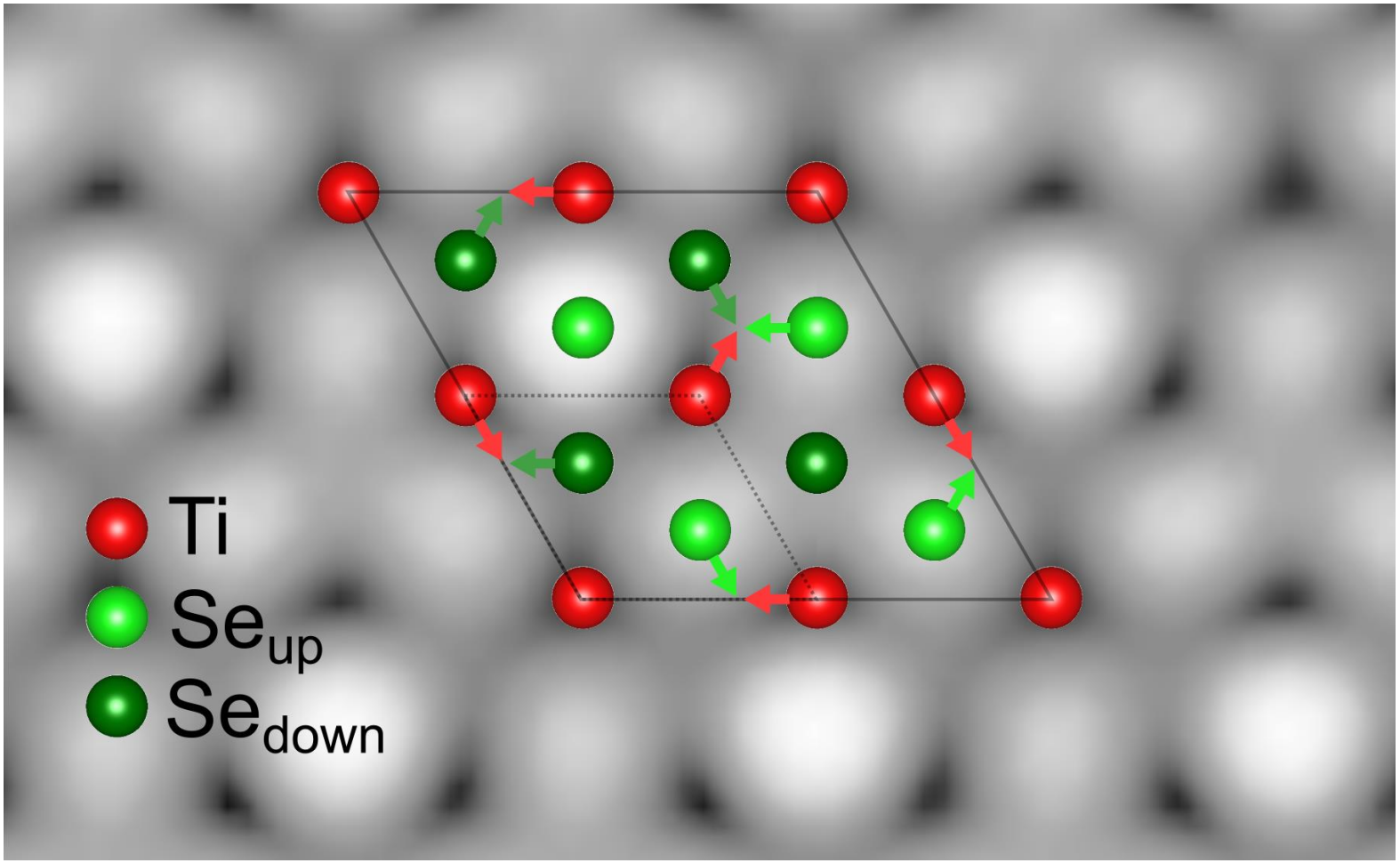
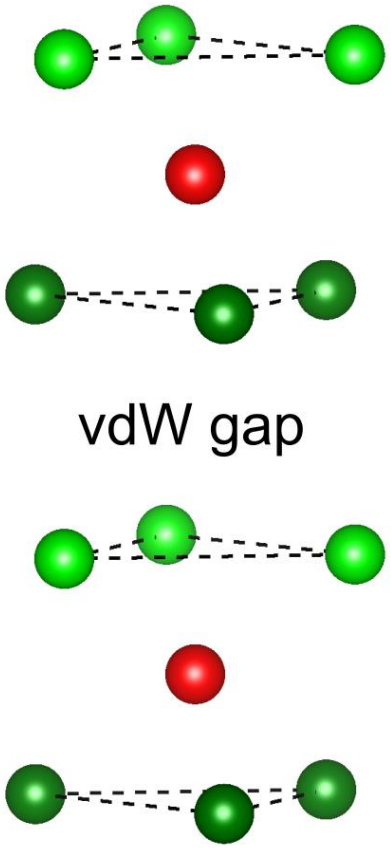


The 3D character of the 1*T*-$TiSe_2$ CDW



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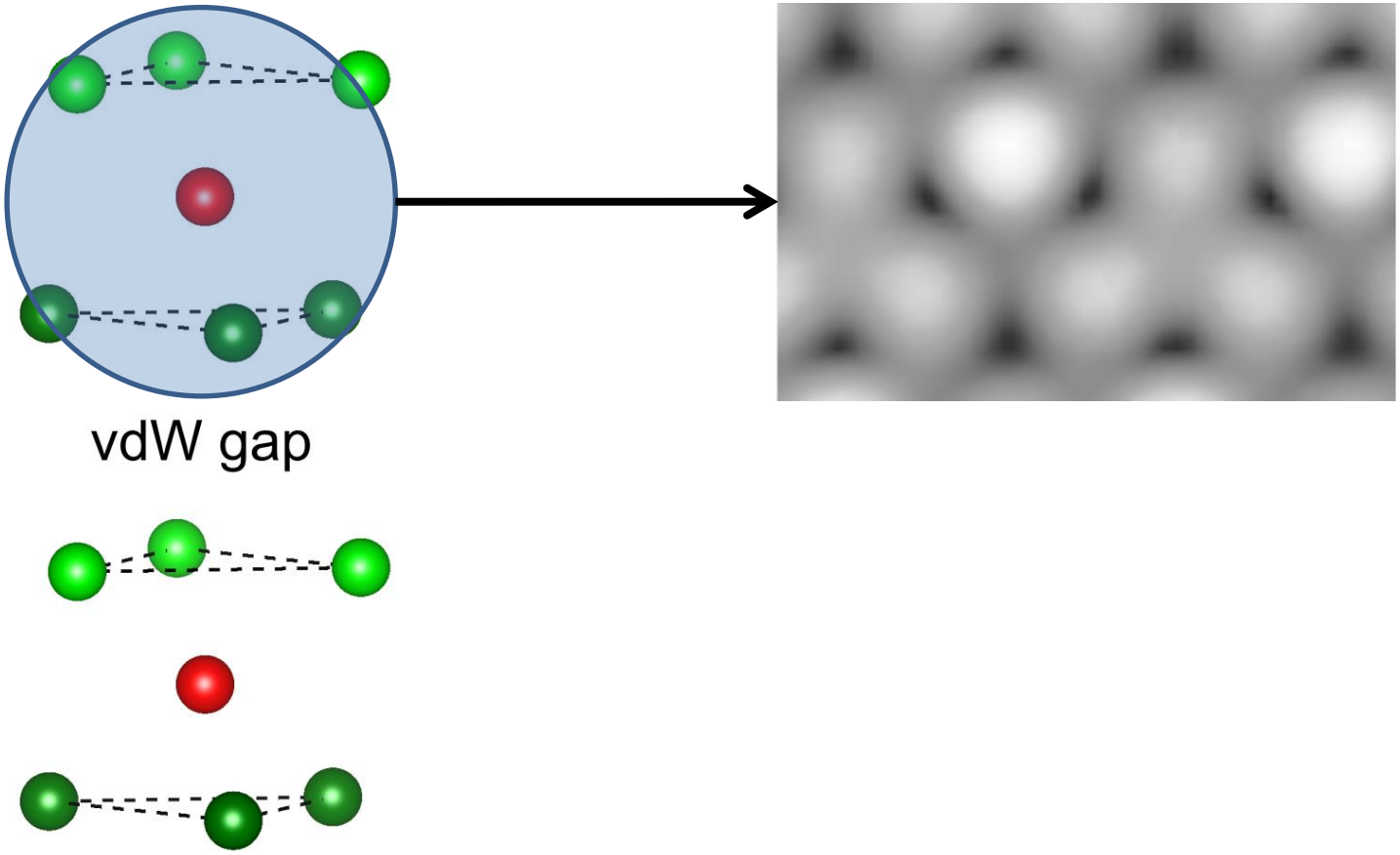

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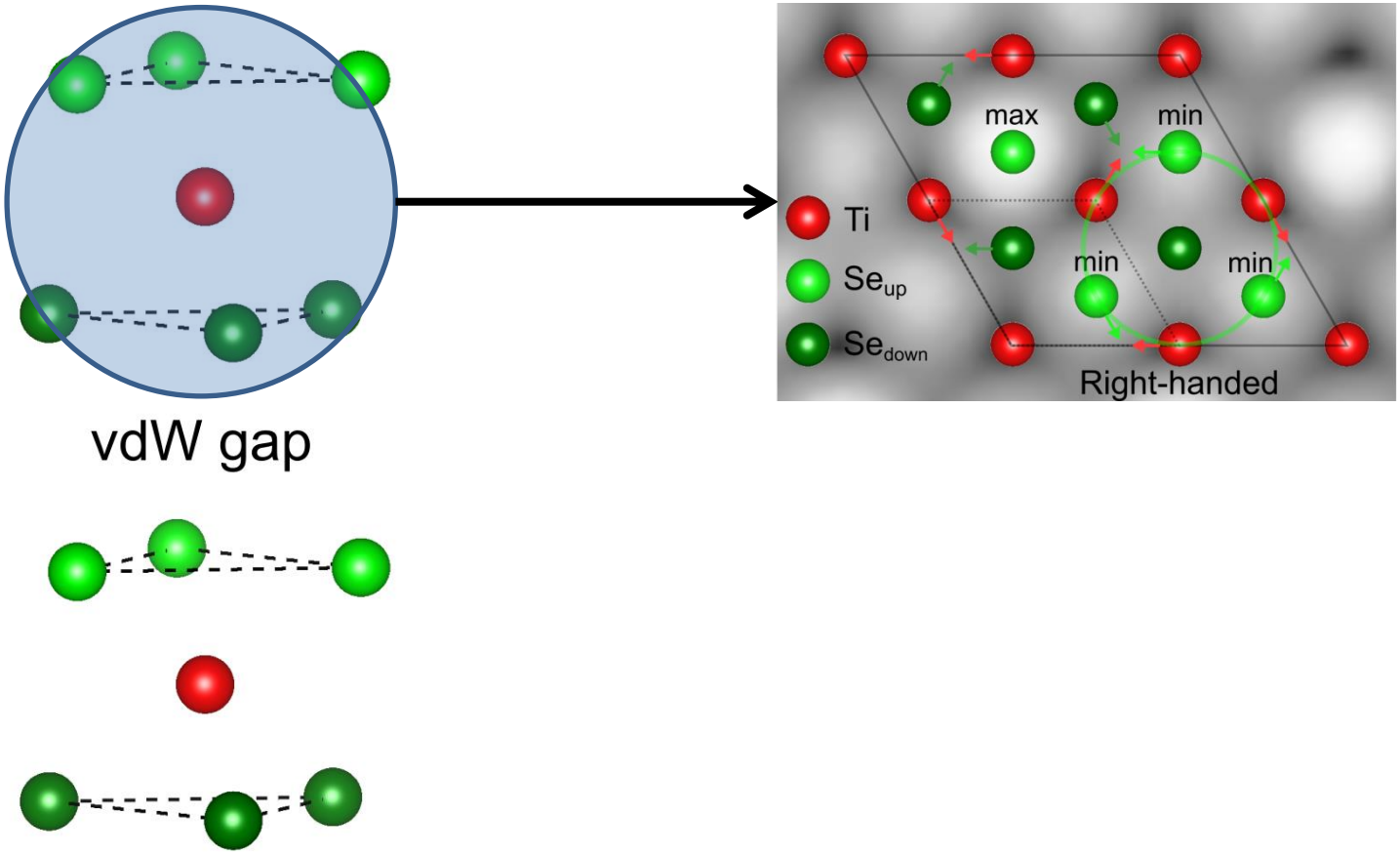

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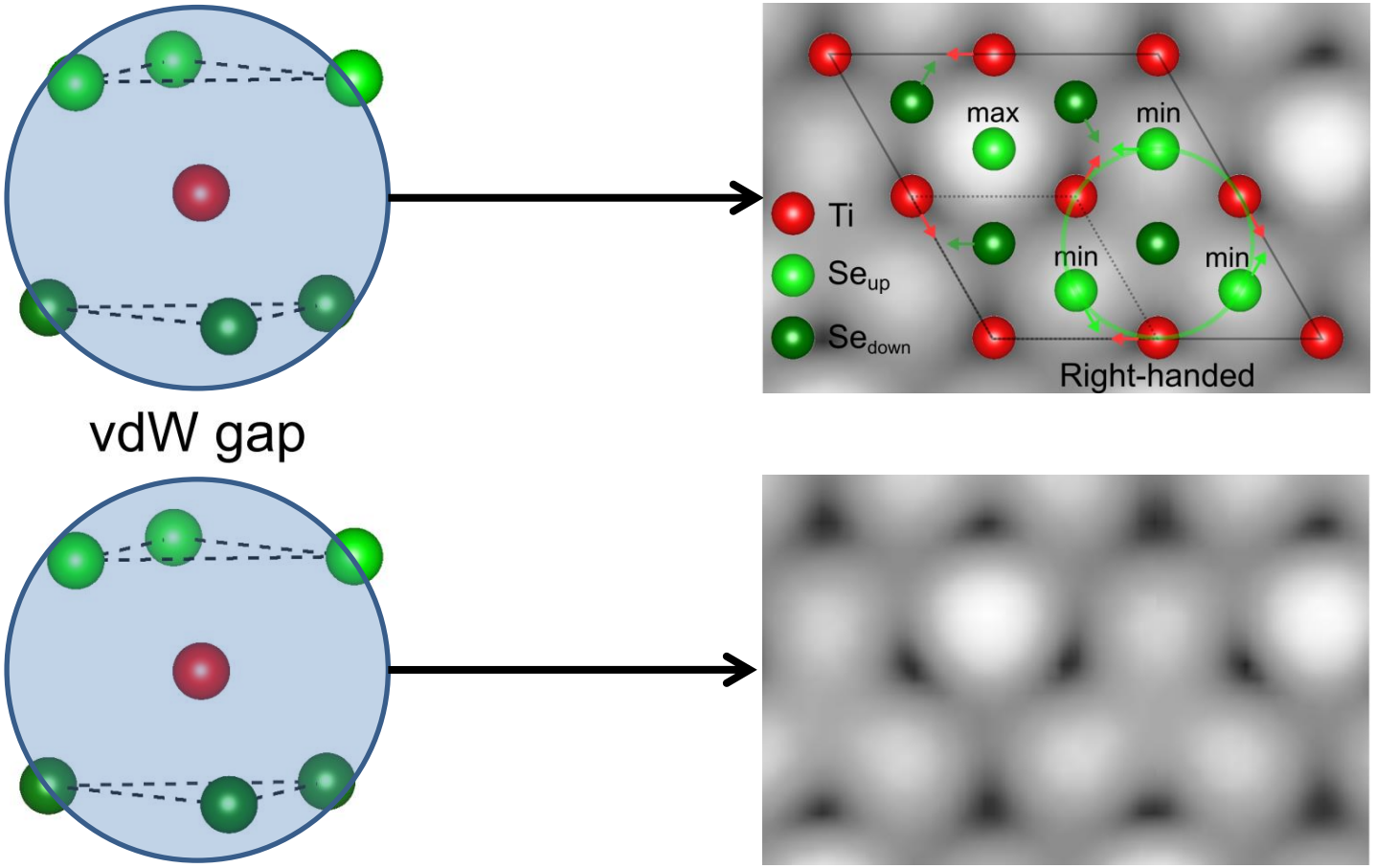

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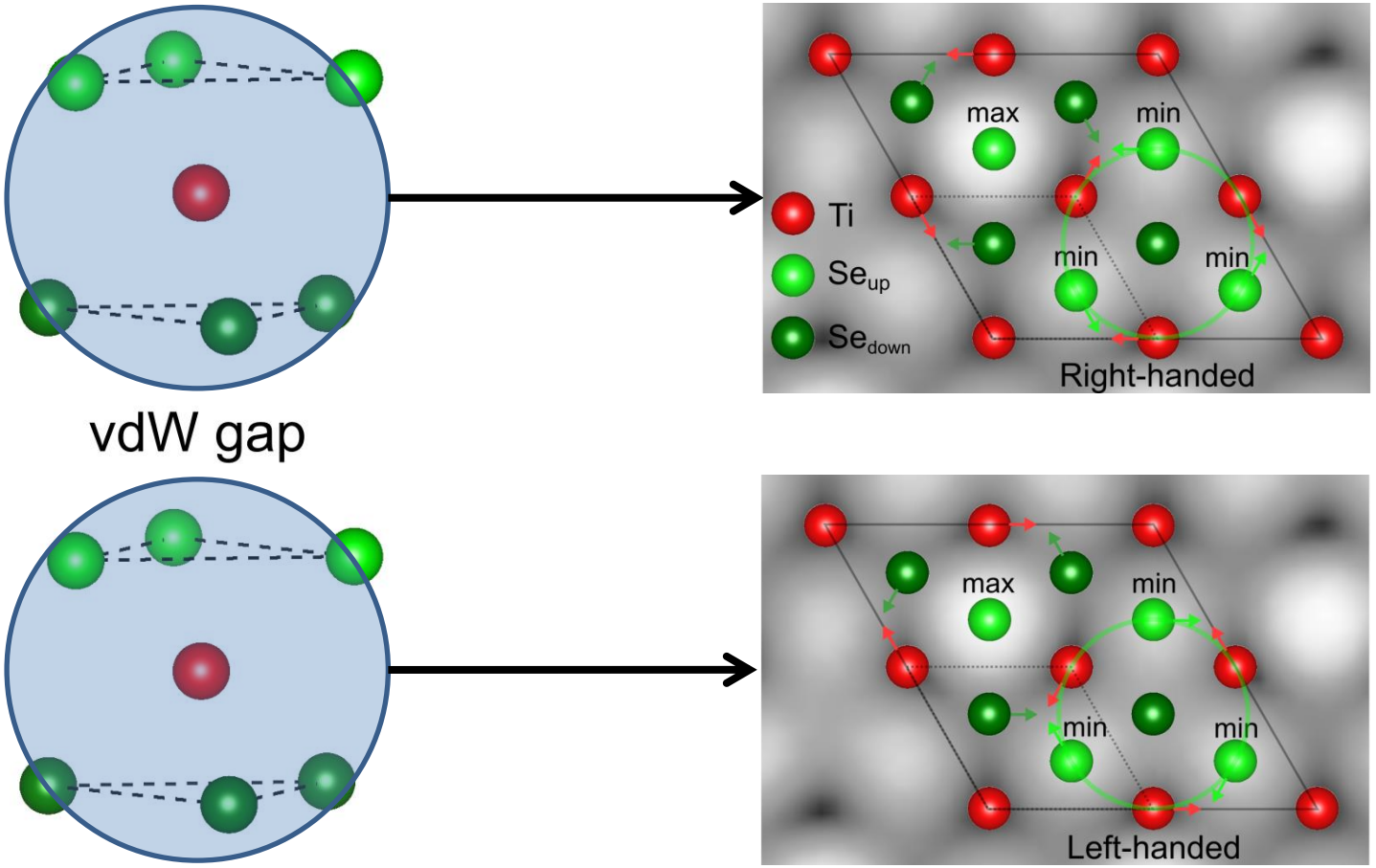

The simple observation of the CDW charge modulation does not allow to discriminate between the two possible PLDs at the surface…

Observation of a new defect

Initial question :

What happens when the density of Ti self-doping is increased above 2.5% ?

→ New samples were grown at 700°C with 5% additional Ti in the tube.

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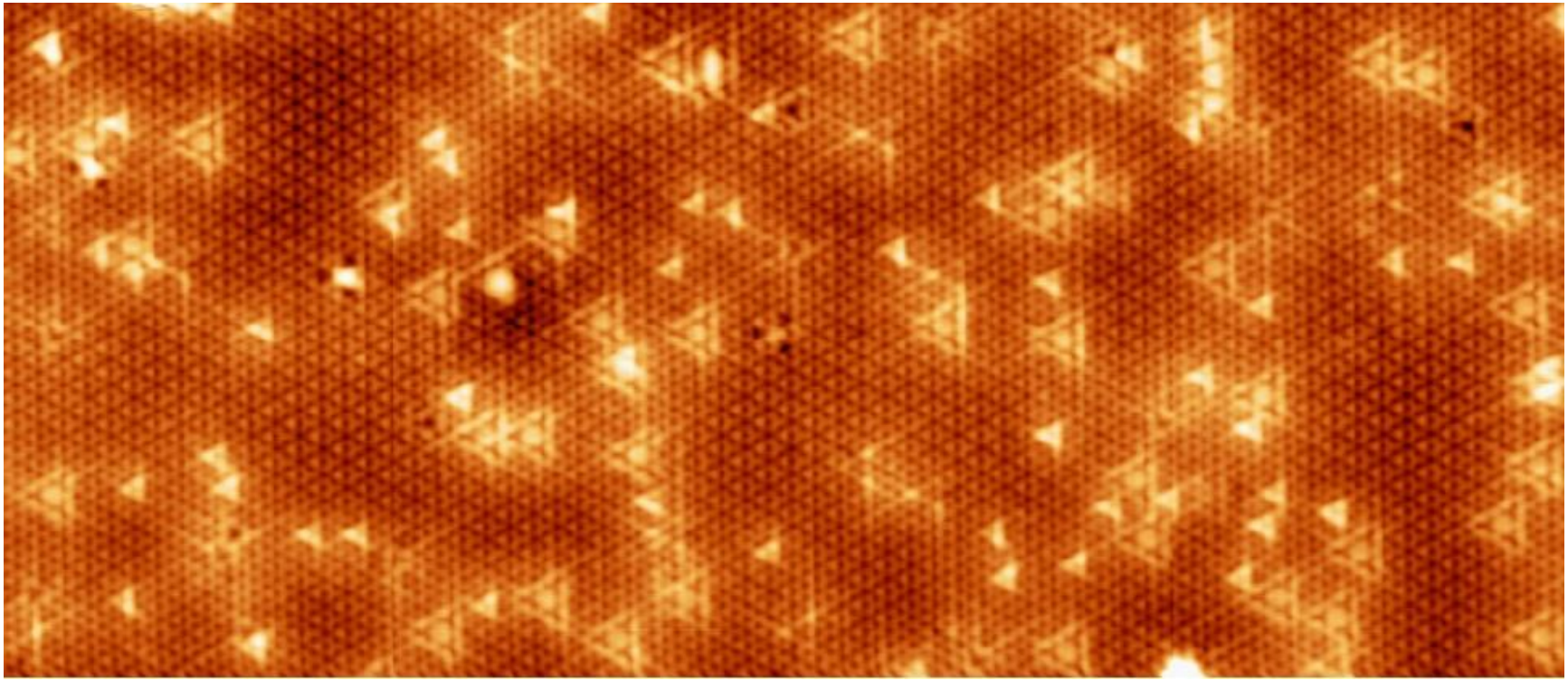

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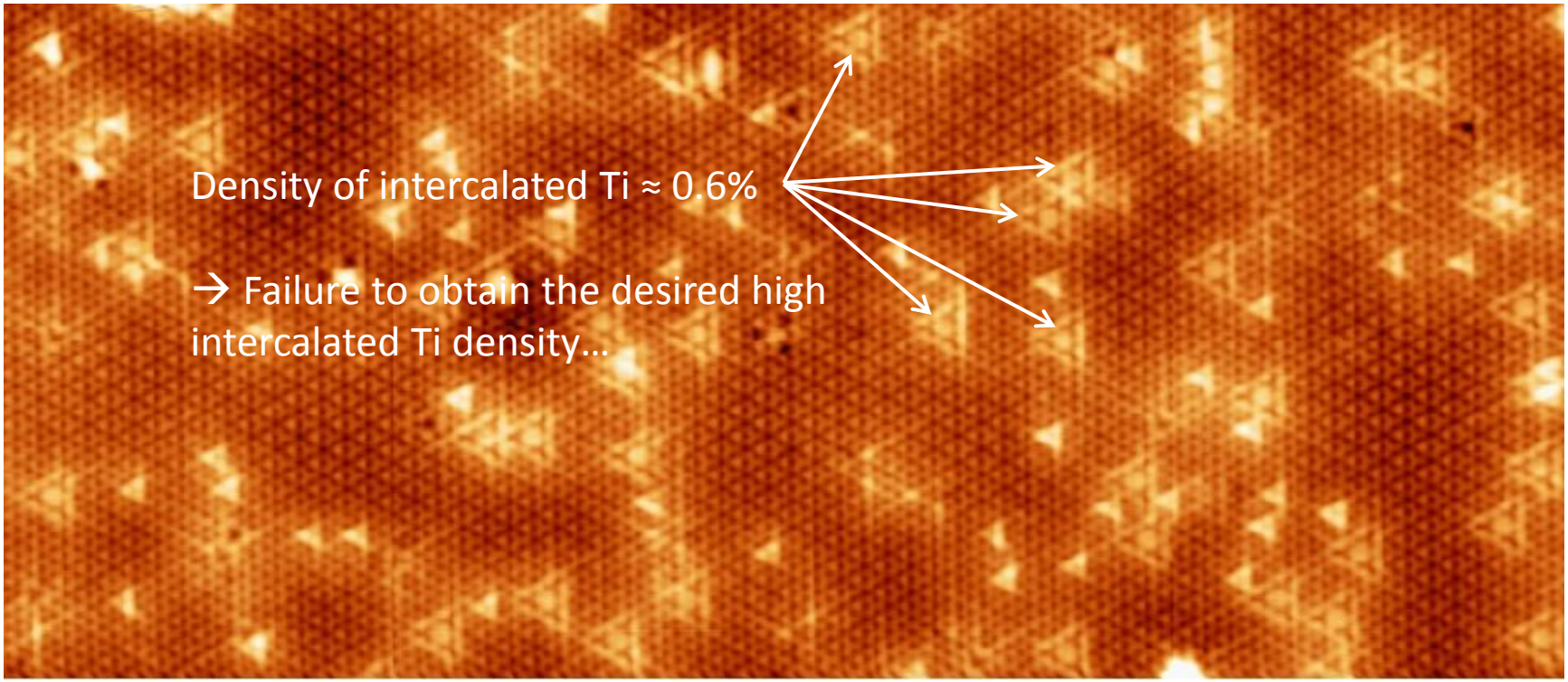

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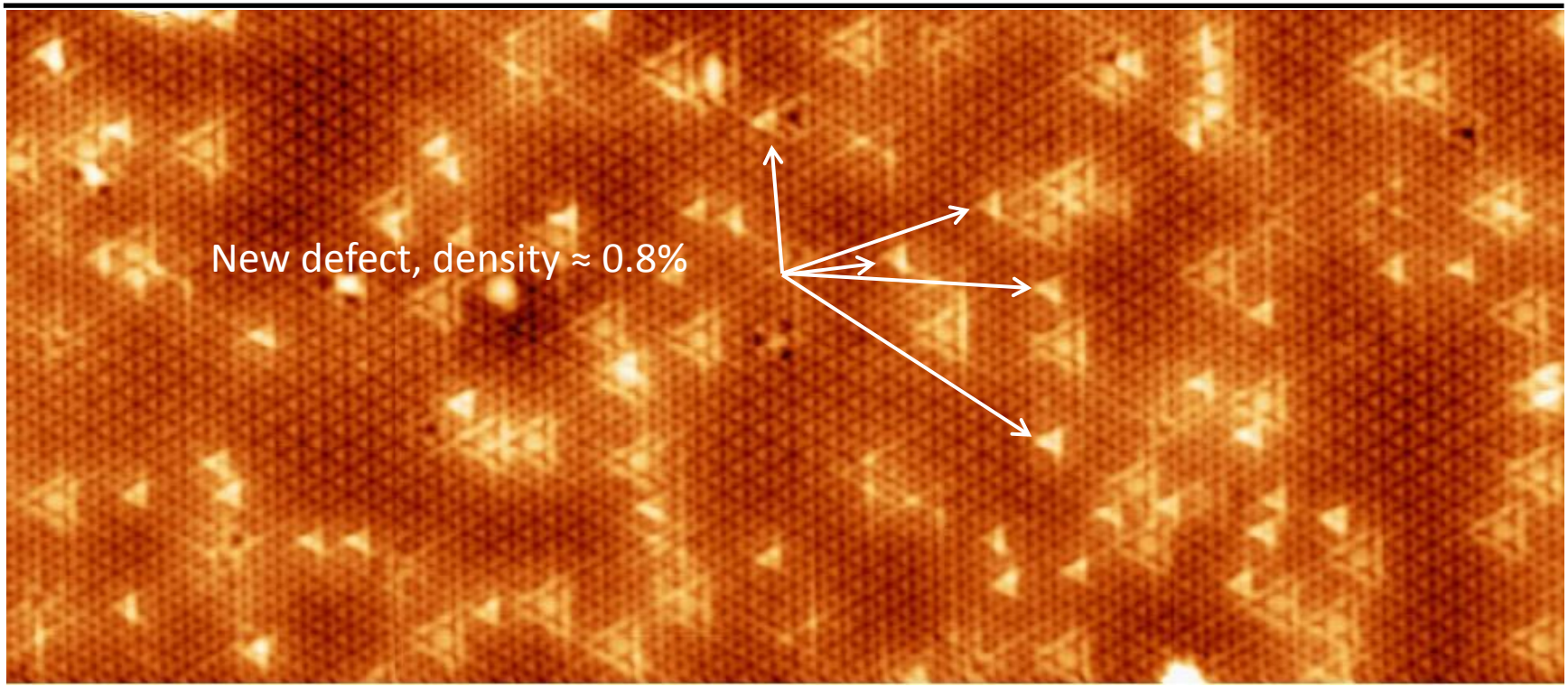

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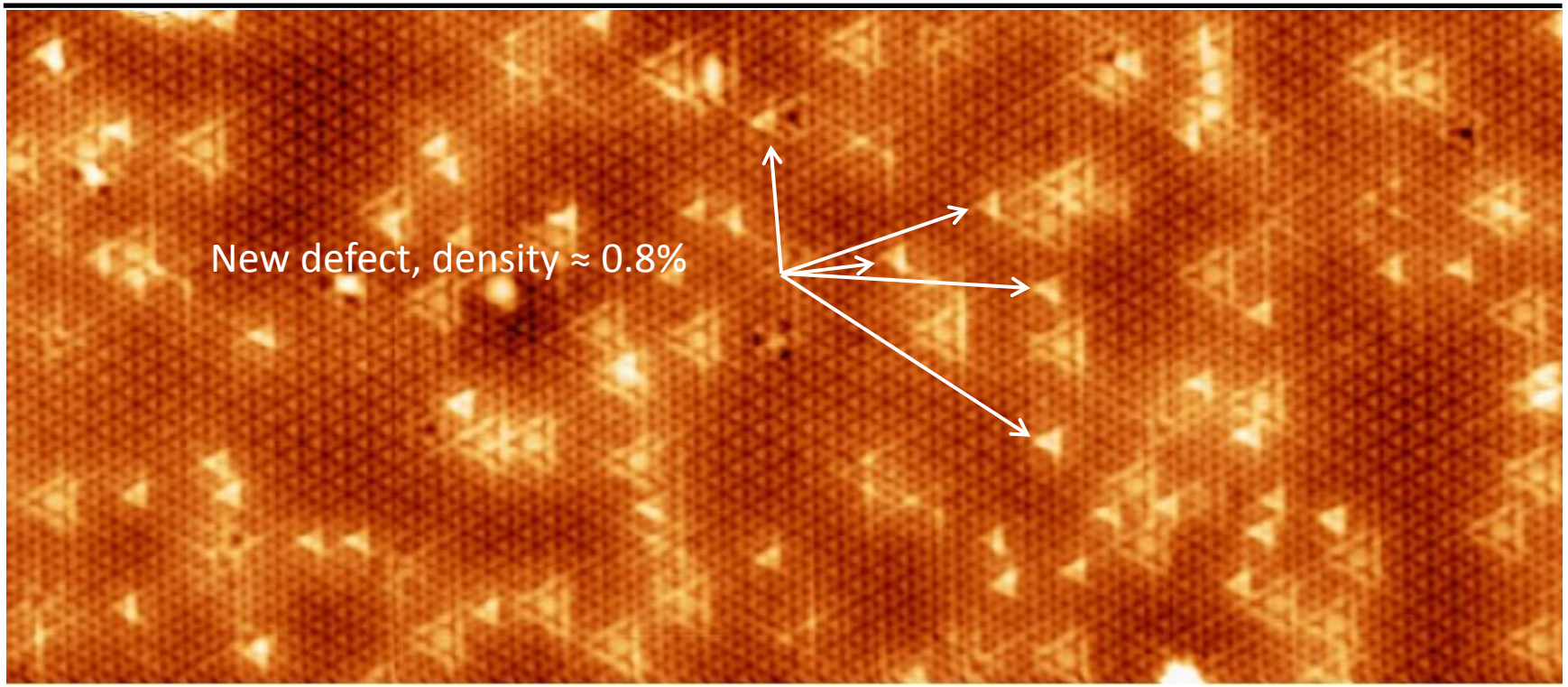
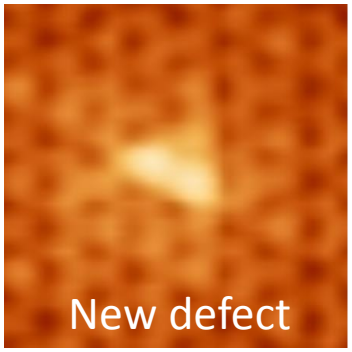
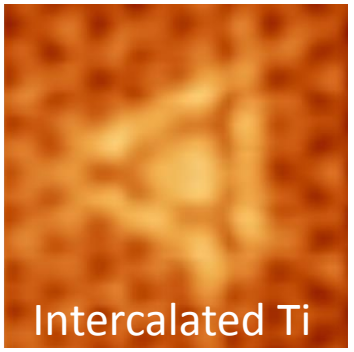


The new defect does not look like intercalated Ti.





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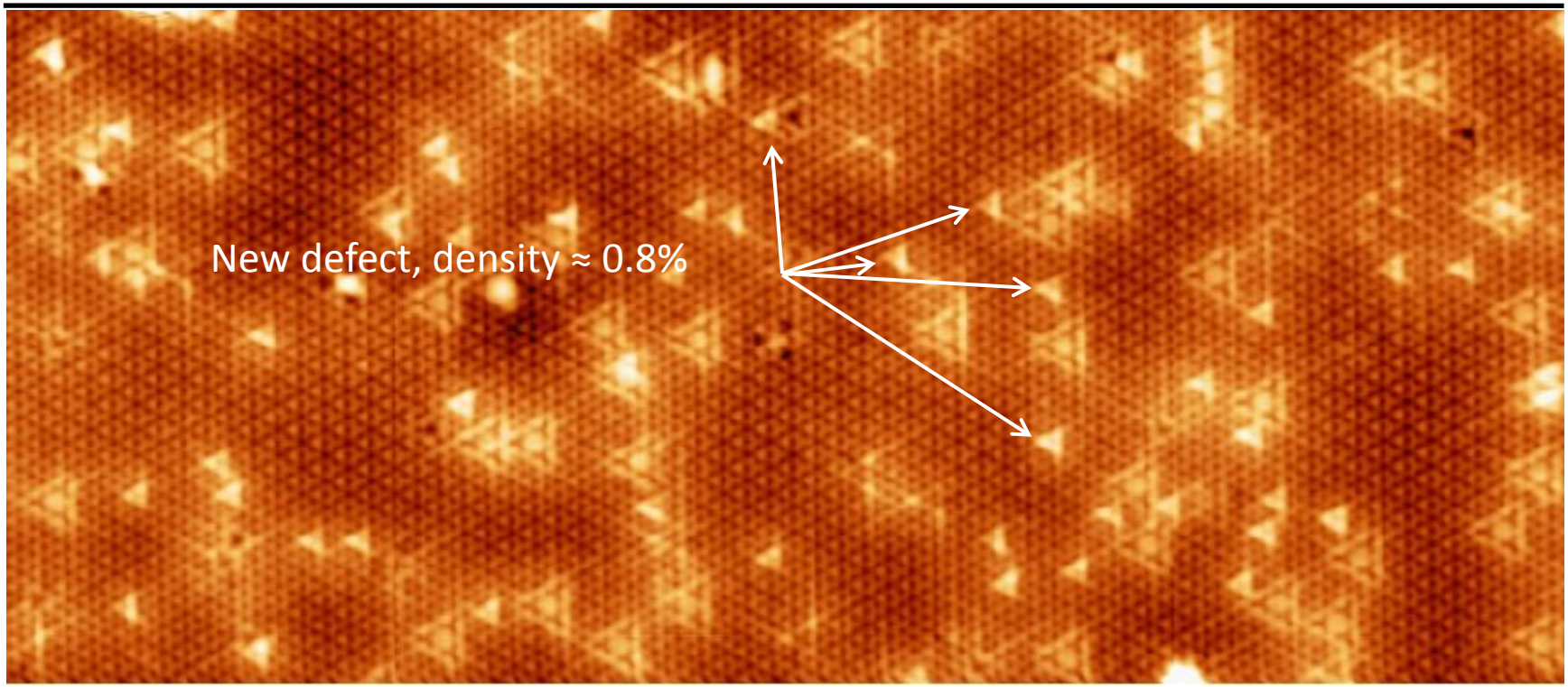
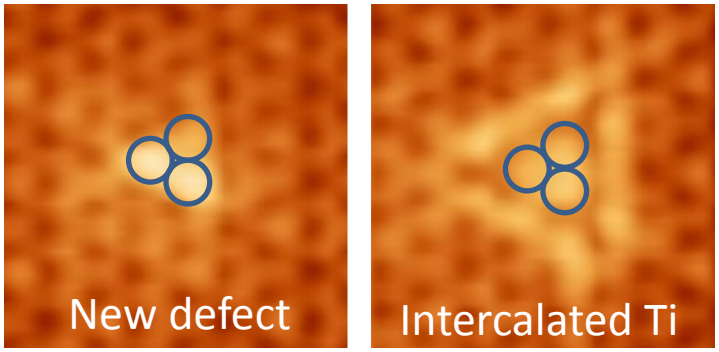


The new defect does not look like intercalated Ti.

But it is placed, such as intercalated Ti, in vertical alignment with a structural Ti.



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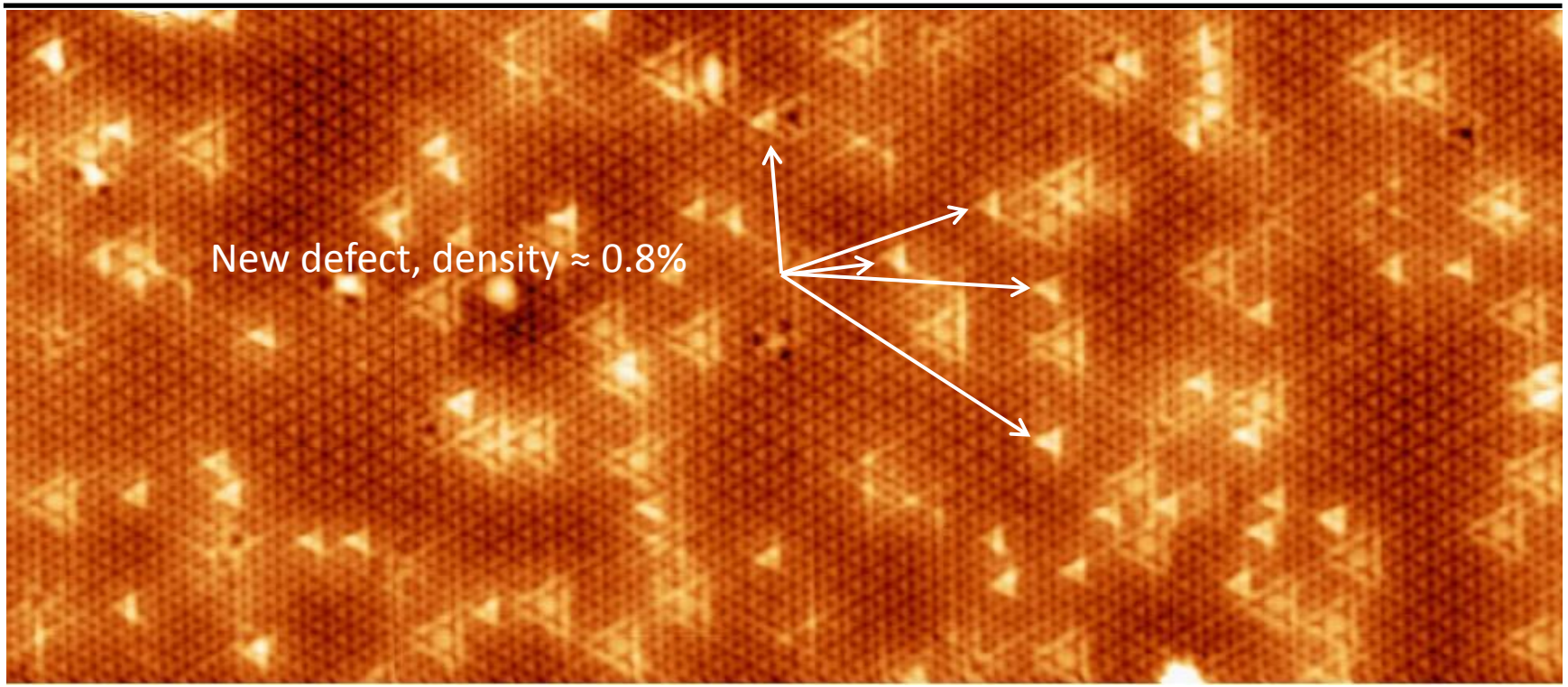

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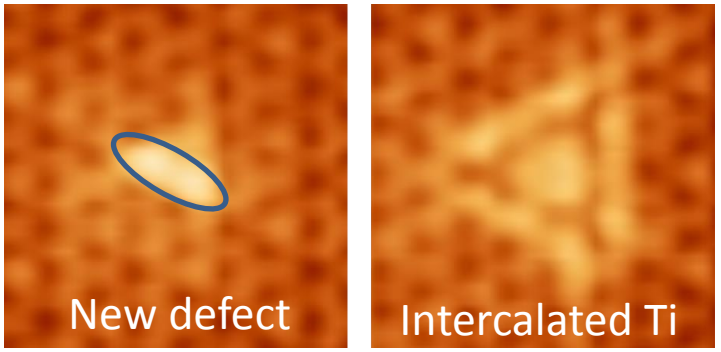
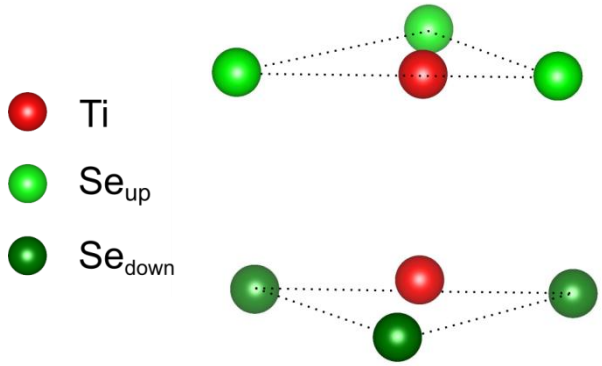
It exhibits a well recognizable **asymmetry** with respect to the CDW, the “bright edge”.



The new defect as a probe of the surface PLD



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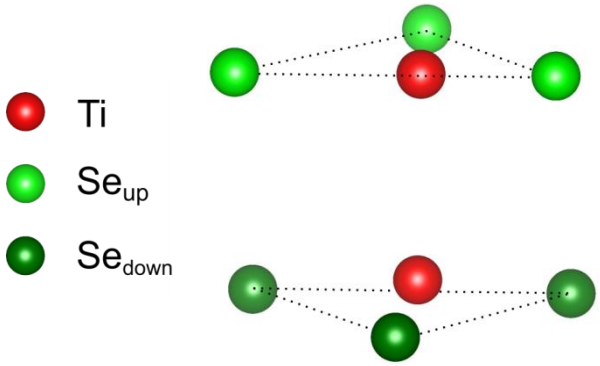

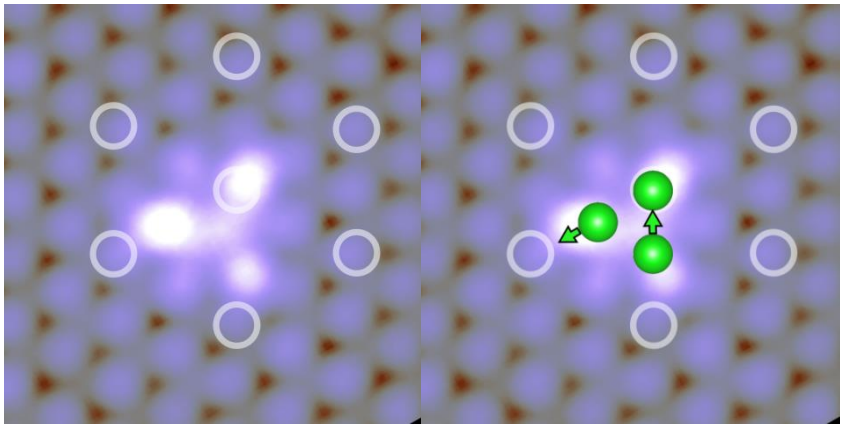

DFT simulation, V_{bias}=0.2 V

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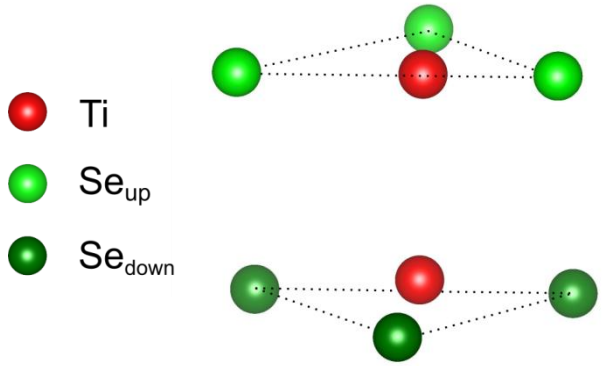

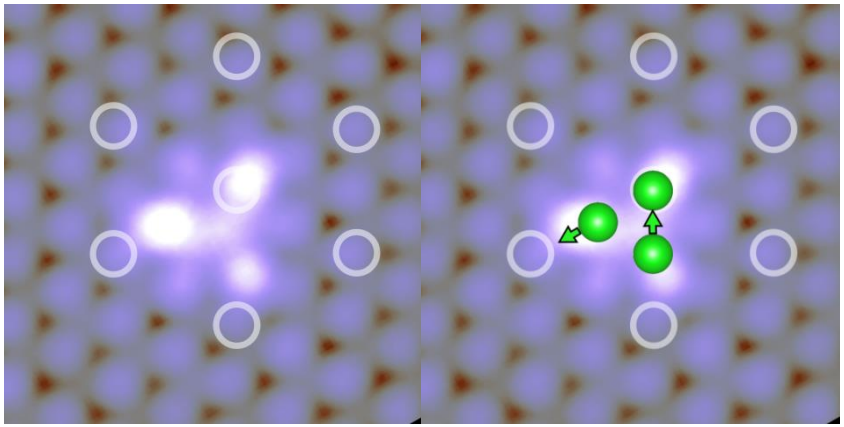

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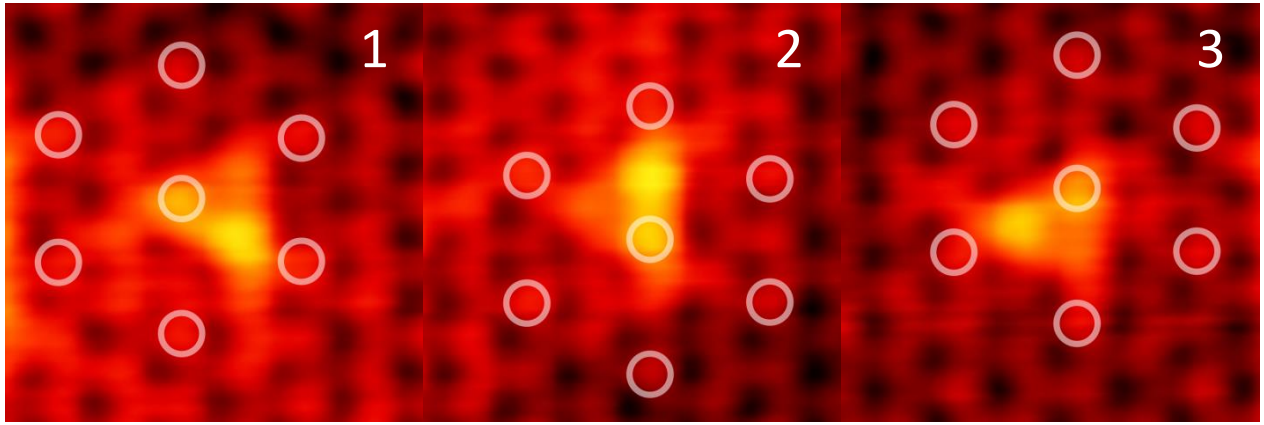

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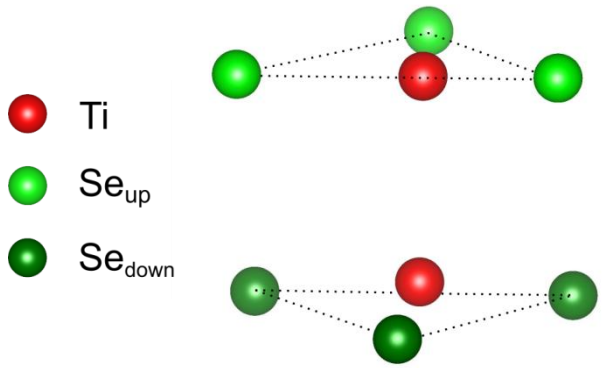

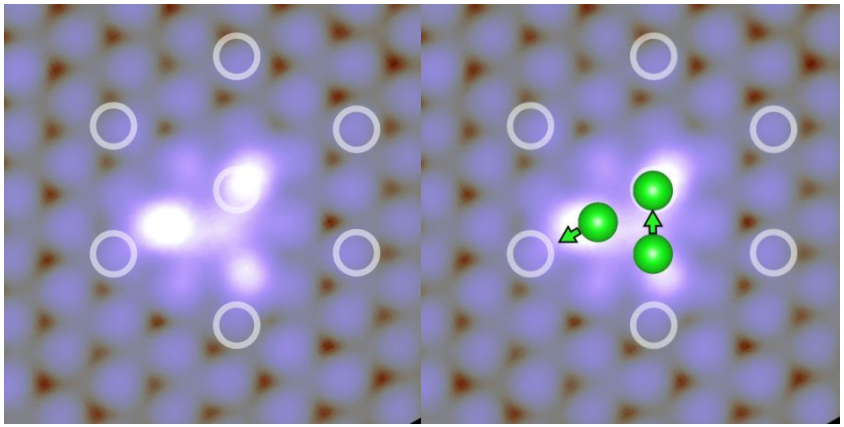

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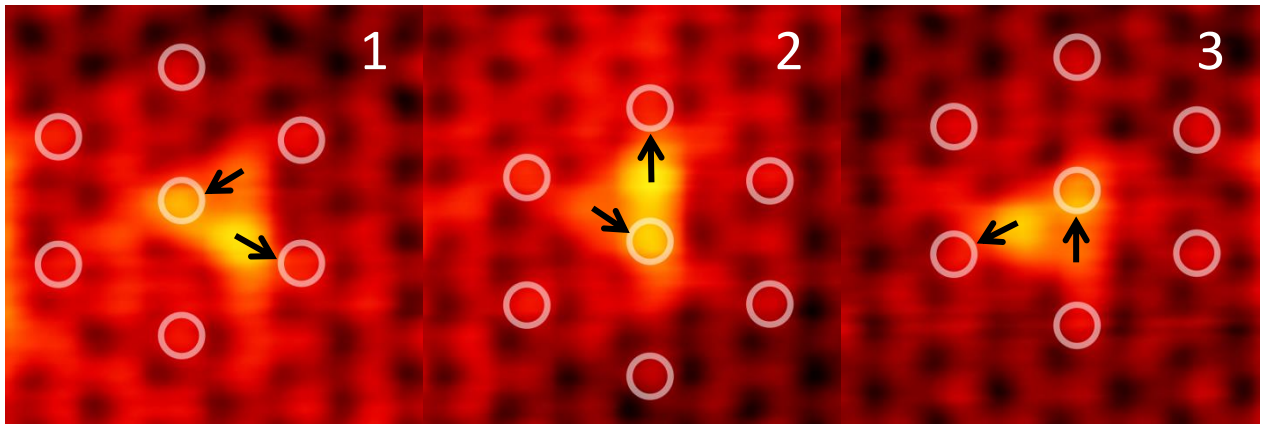
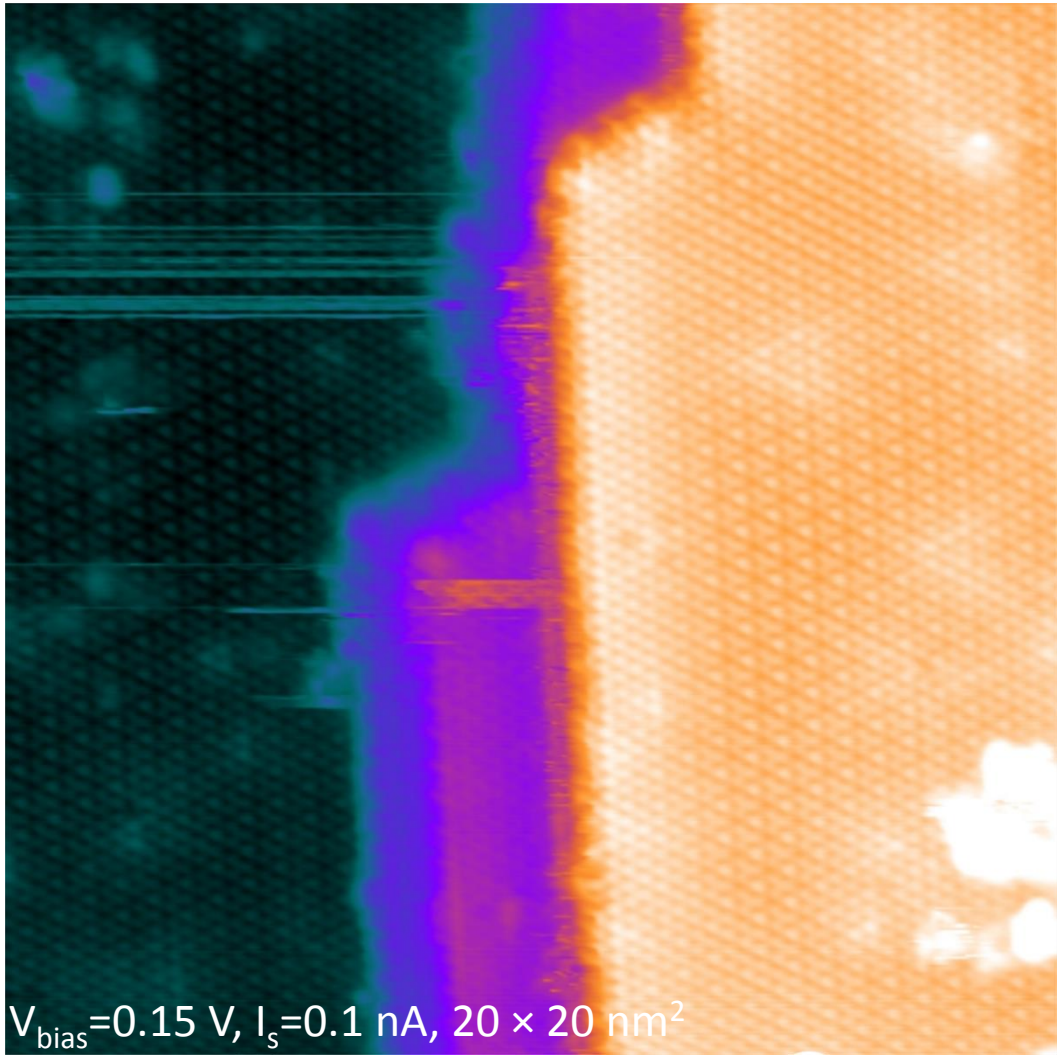


Right-handed !

It is therefore possible to probe the symmetry of the PLD using this new defect

Strength of method tested on a step edge



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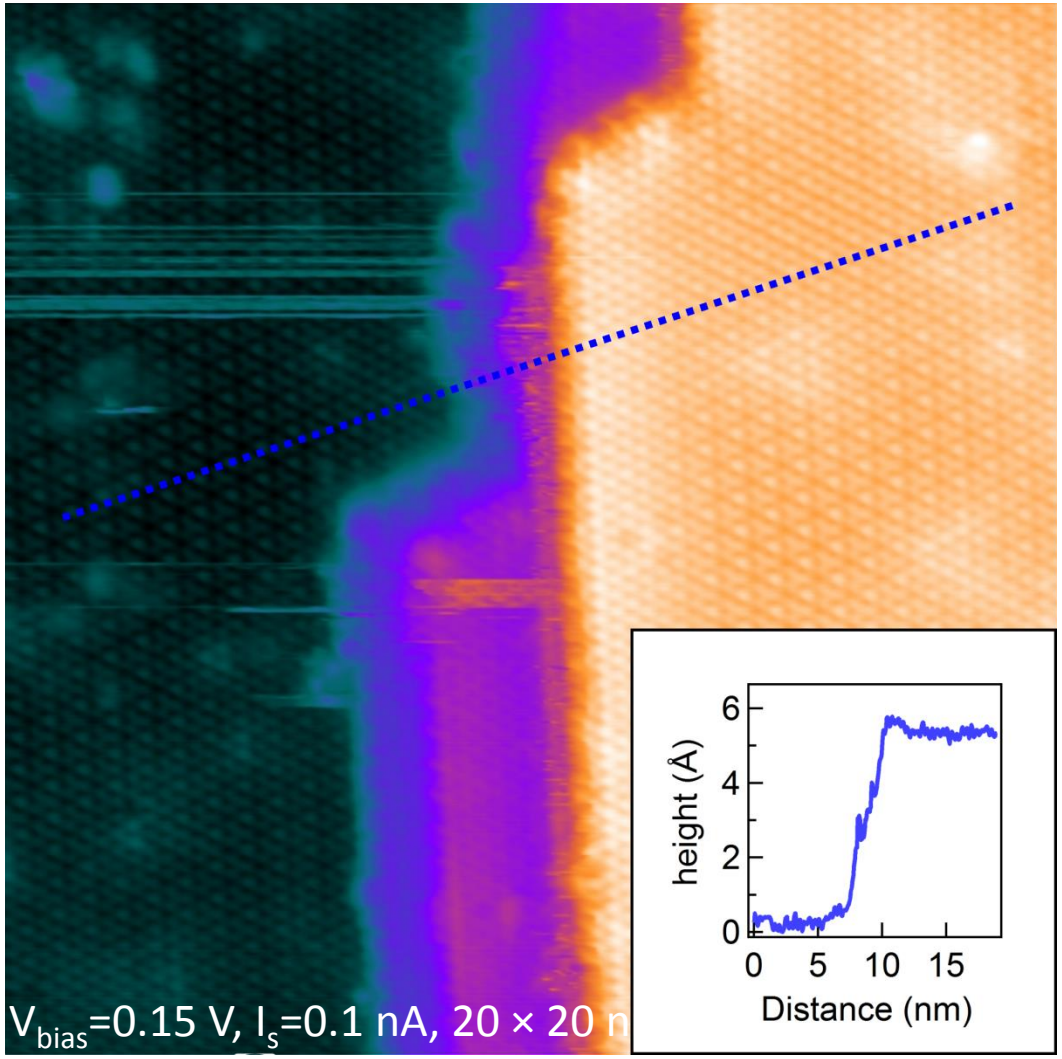

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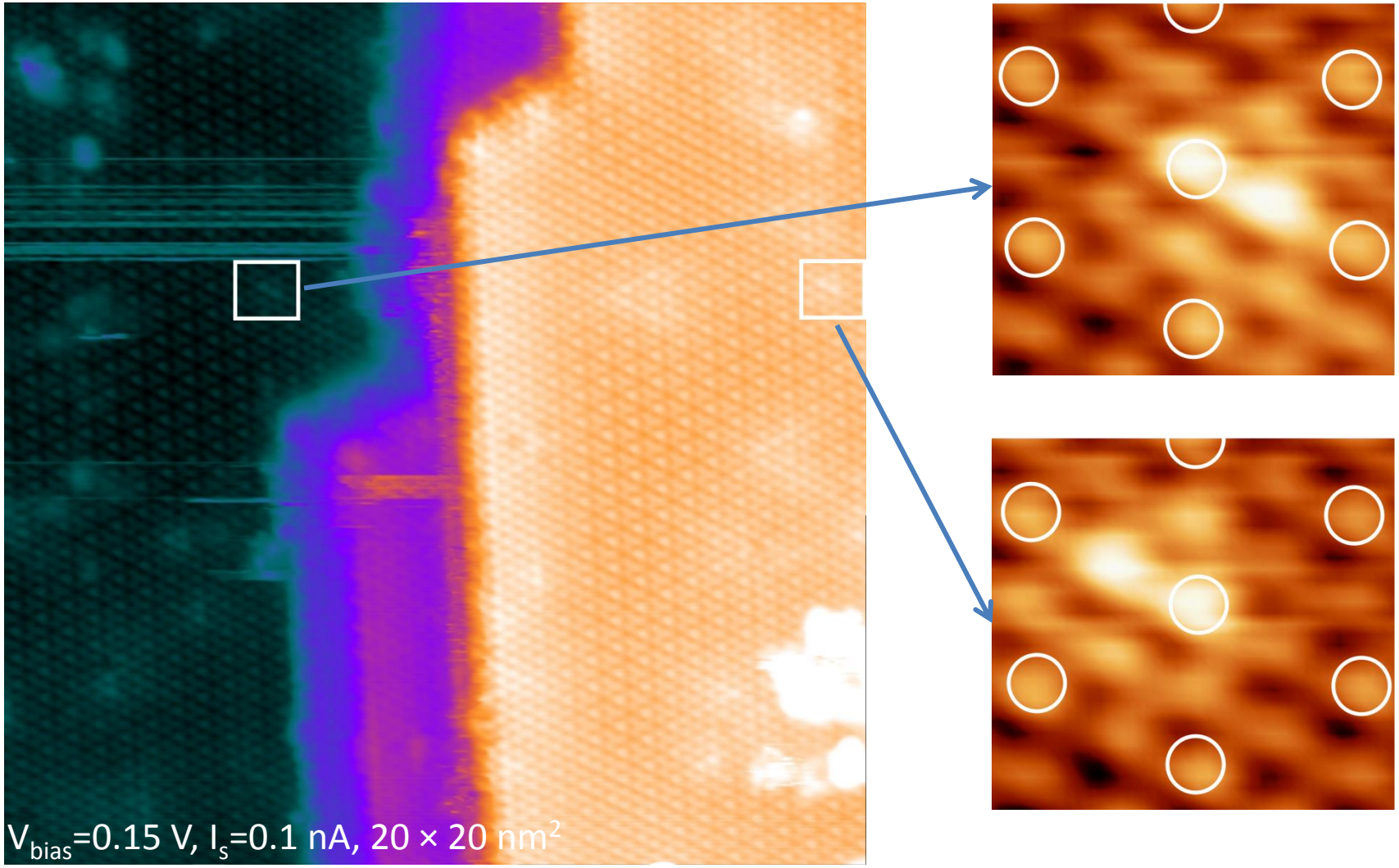

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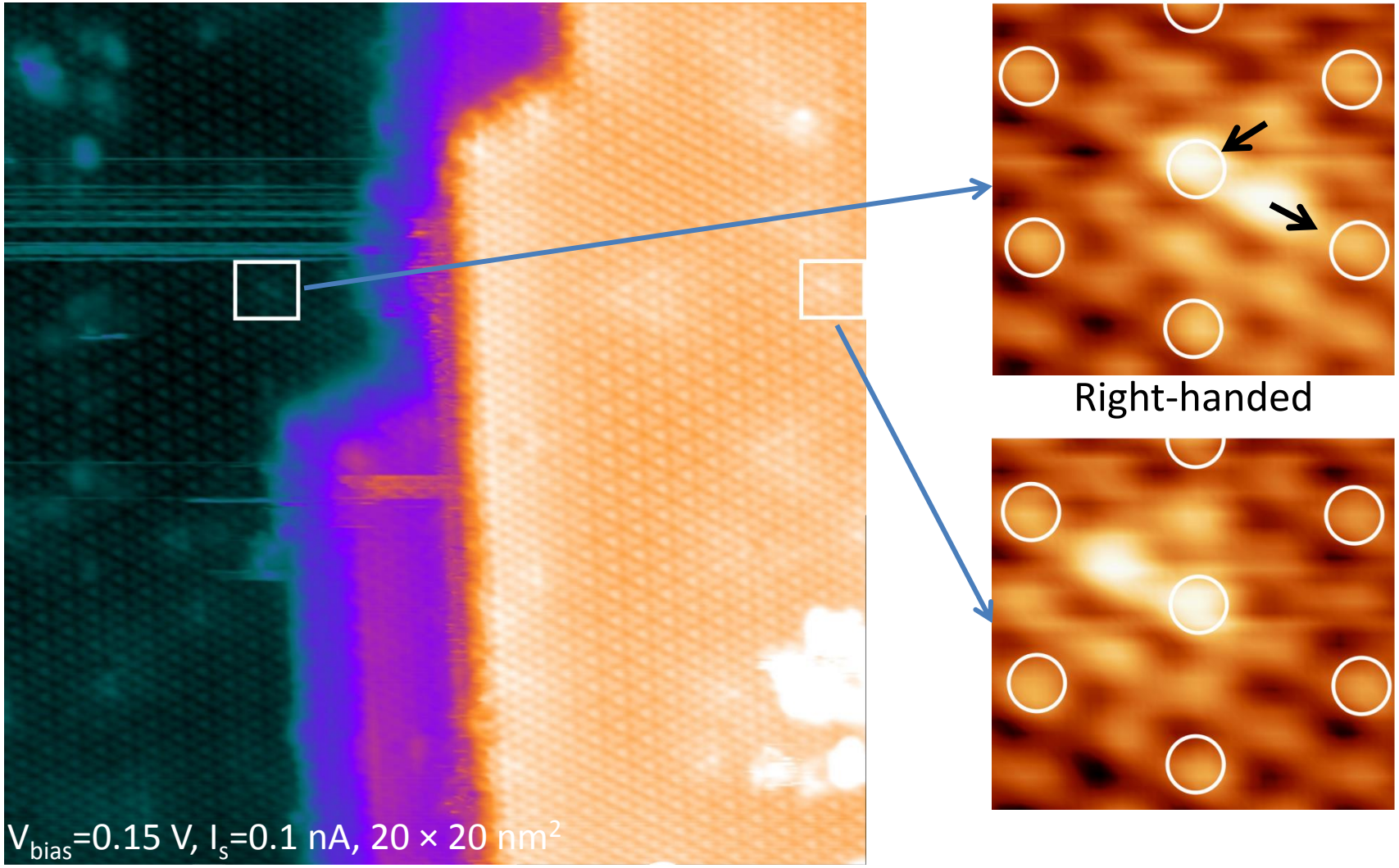

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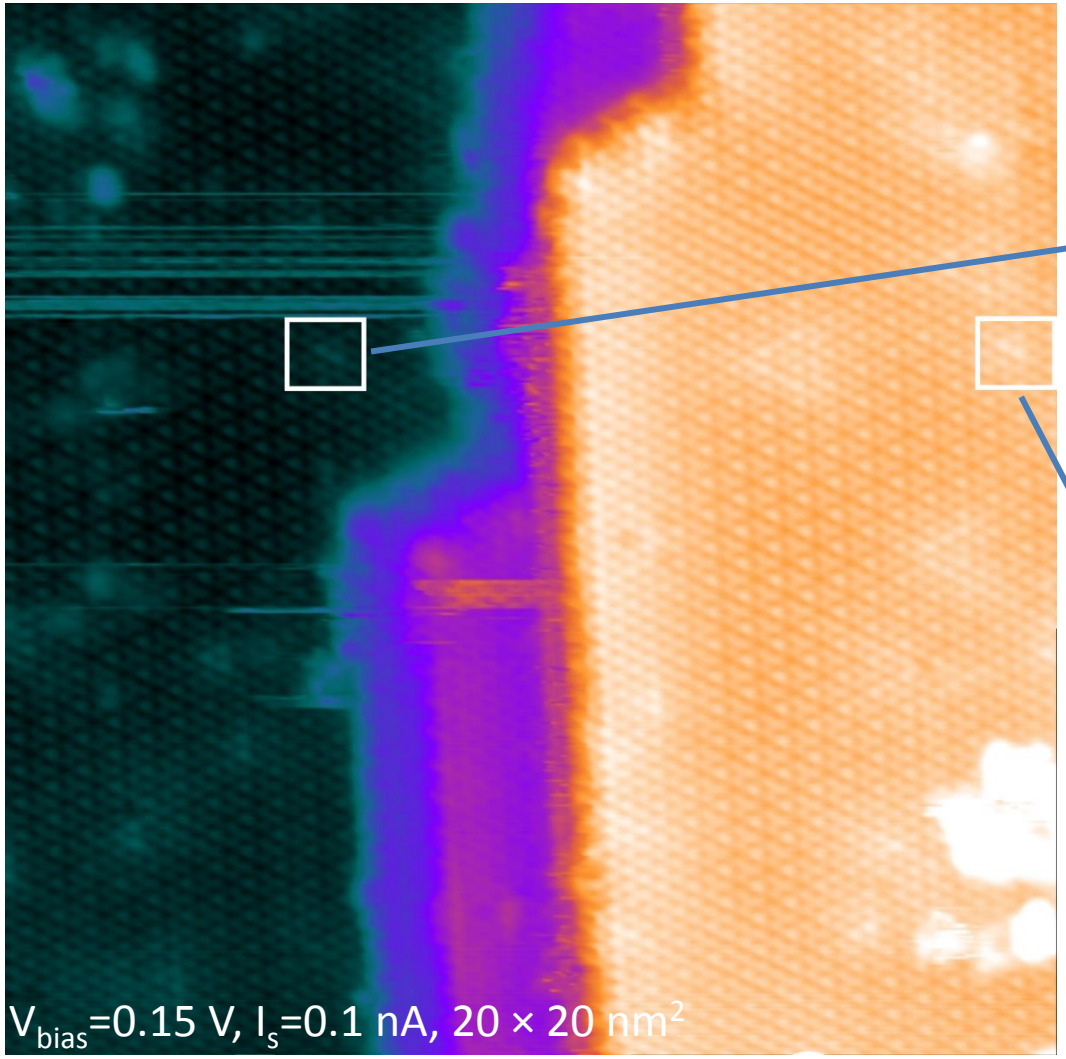
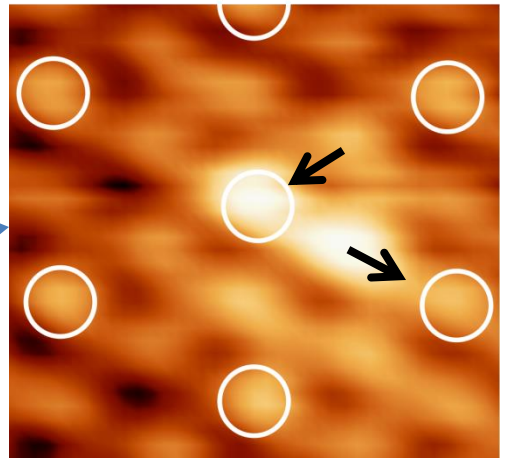
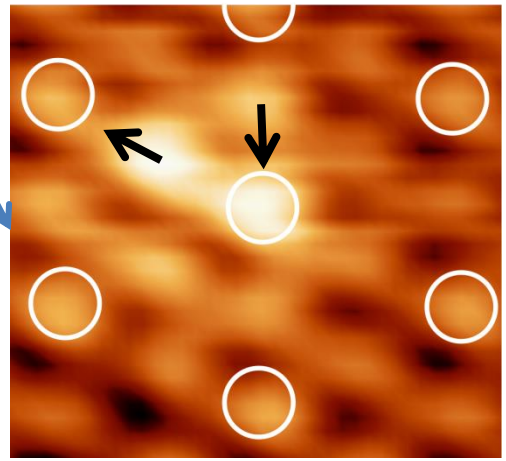




Right-handed



Left-handed

This observation confirms that the CDW is 2 x 2 x 2 on this sample !

Outlook

Probe the underlying PLD in the presence of doping-induced domains (Cu and Ti) .

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Consider the third dimension in the topic of chirality.