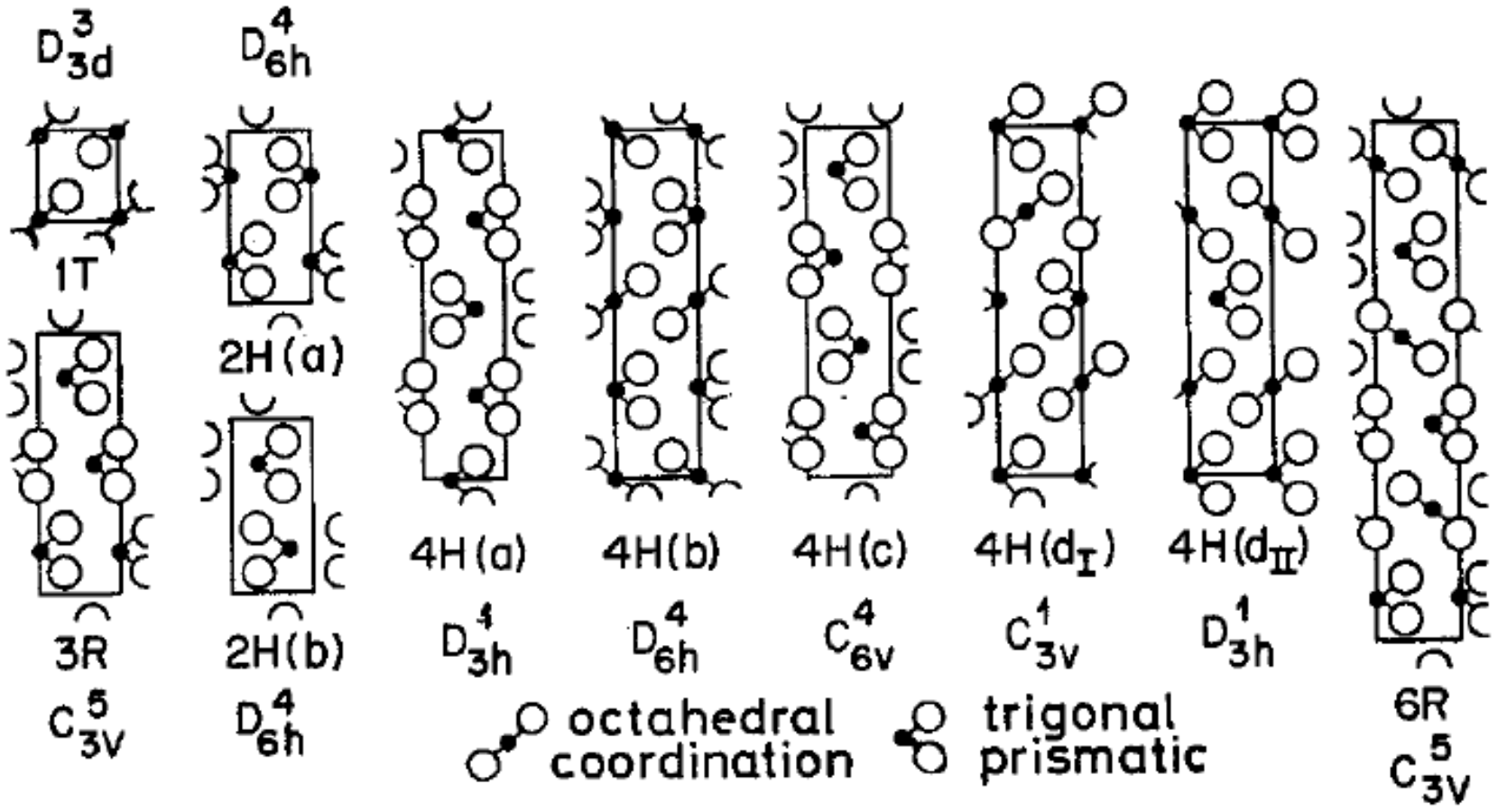
Курс: Електронна структура та властивості низькорозмірних систем

Лектор: Олександр Кордюк

Лекції 5-6: **Хвилі зарядової густини в дихалькогенідах перехідних металів та квазікристали**

- Transition metal dichalcogenides: composition, structure, and applications
- Квазідвовимірність та електронна структура
- CDW in $TaSe_2$: переходи у співрозмірну на неспіврозмірну фази, псевдощілина
- Нестинг, автокореляція та двохчастинкова спектральна функція
- Commensurate vs Incommensurate…
- CDW band gaps
- Плитки Пенроуза та квазікристали

CDW in transition metal dichalcogenides

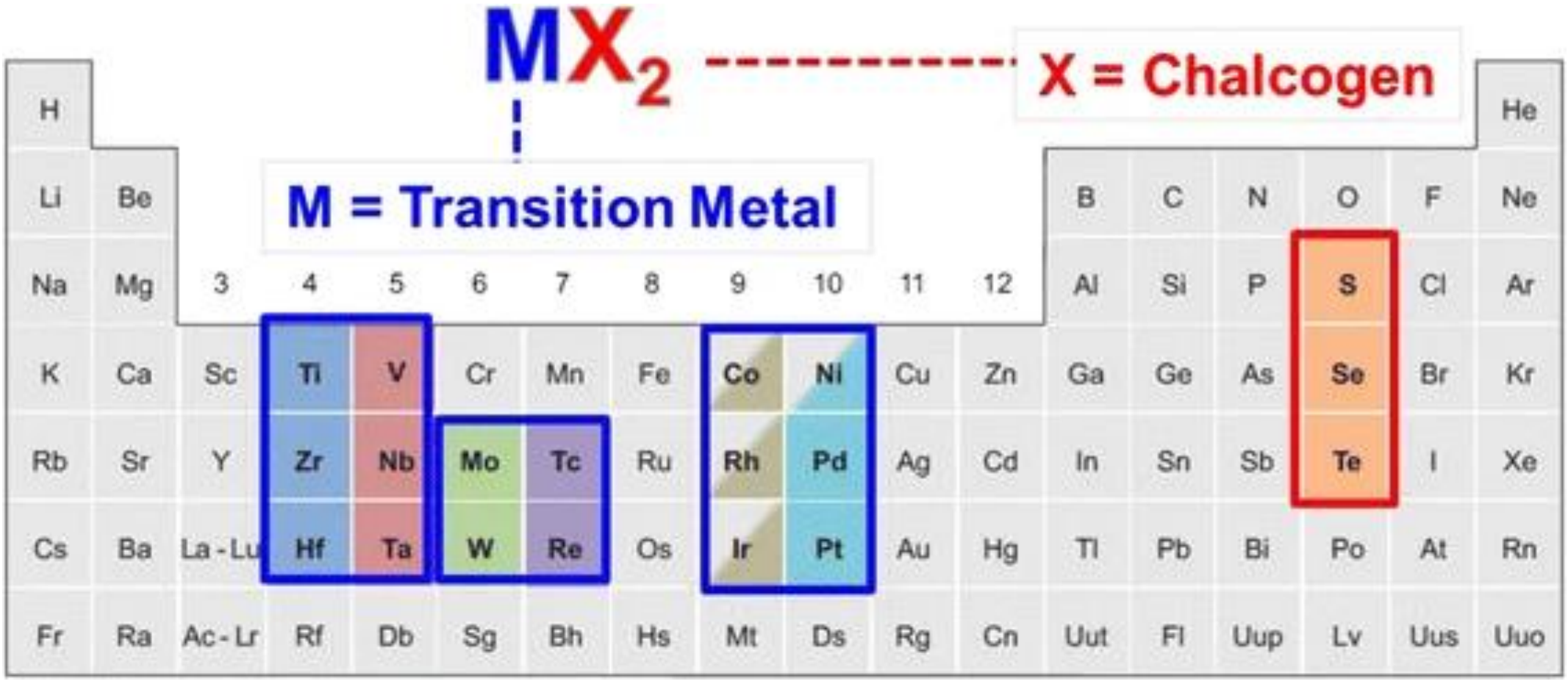


Various polytypes of the layer structure transition metal dichalcogenides

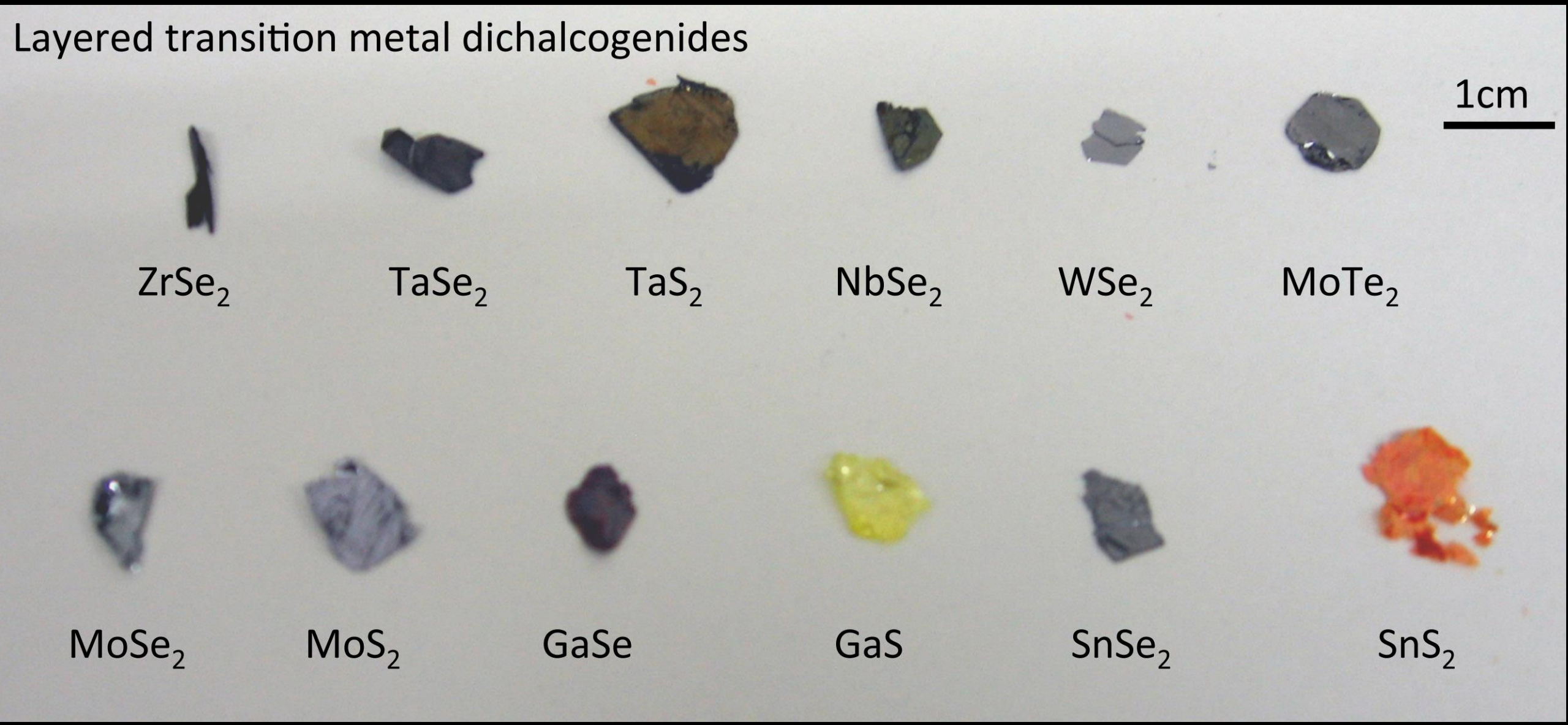
J.A. Wilson & A.D. Yoffe, Advances in Physics (1969)

https://doi.org/10.1080/00018736900101307

Transition metal dichalcogenides

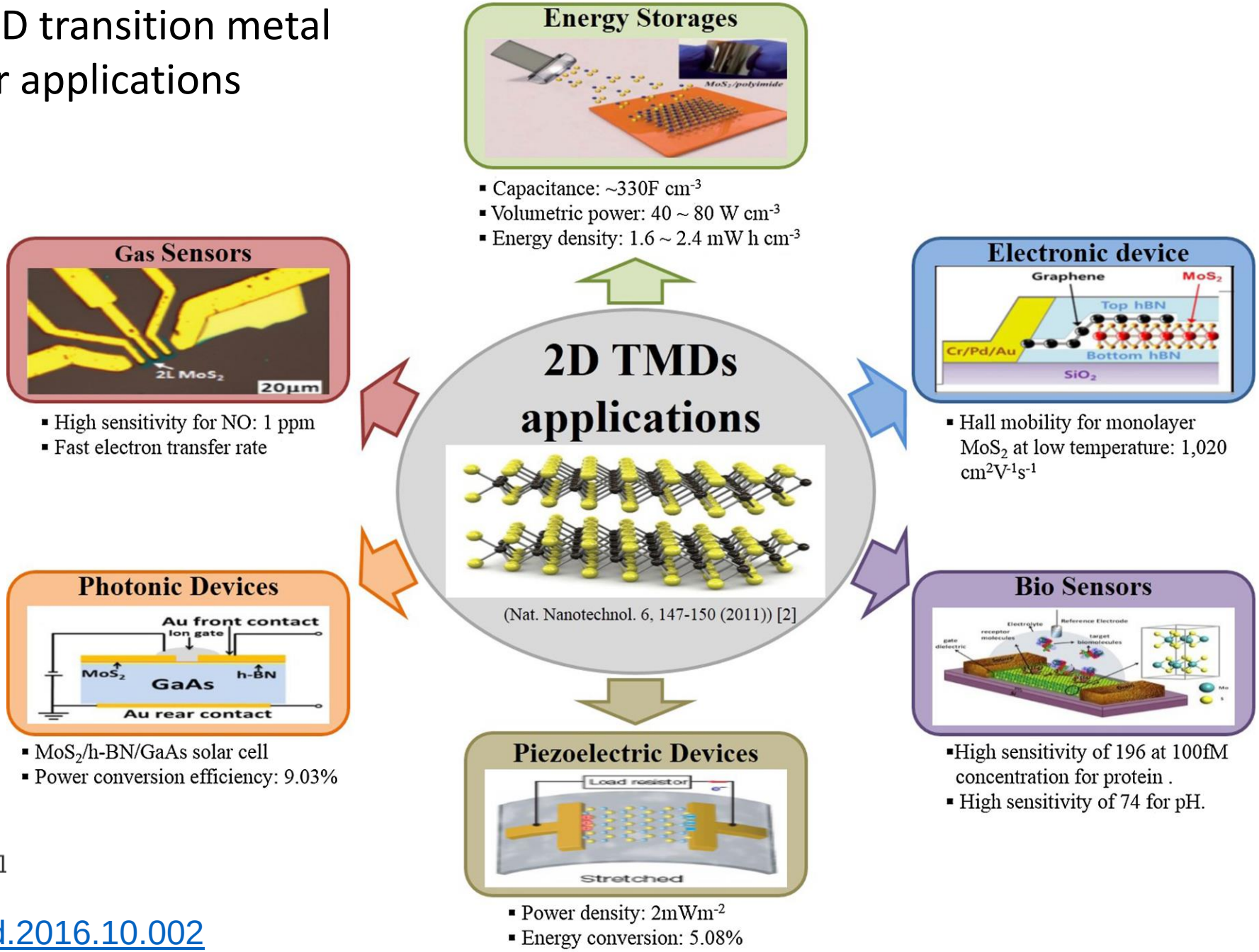


Nano Convergence **2**, 17 (2015)



Various transition metal dichalcogenides (T. Shimada) http://van-der-waals-epitaxy.info/?attachment_id=317

Recent development of 2D transition metal dichalcogenides and their applications



materialstoday
Volume 20, Issue 3, April 2017, Pages 116-1

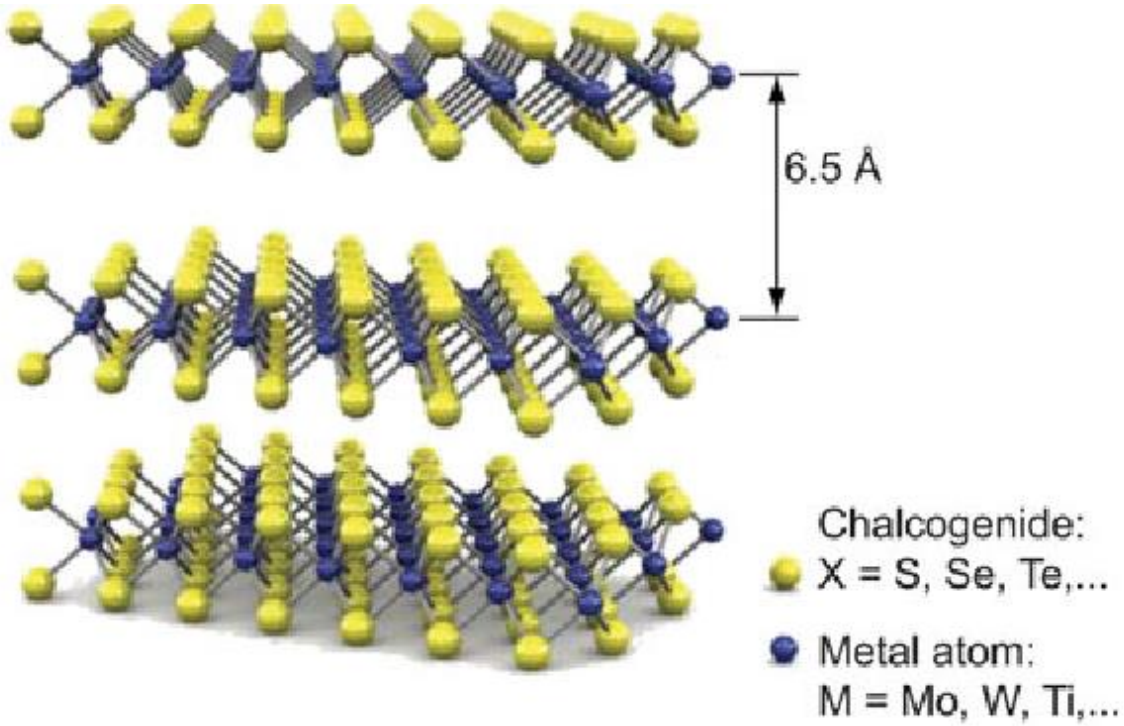
https://doi.org/10.1016/j.mattod.2016.10.002

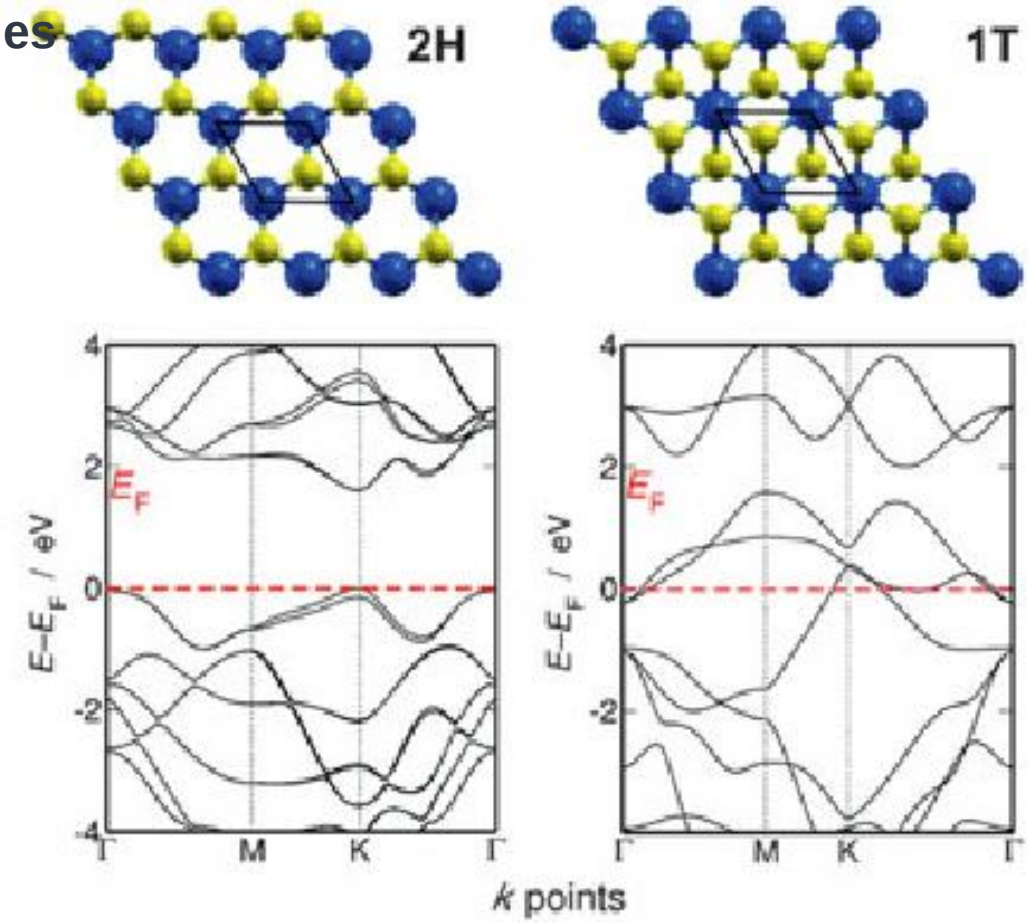
Transition metal dichalcogenides: crystal structure

Electronic properties of transition-metal dichalcogenides

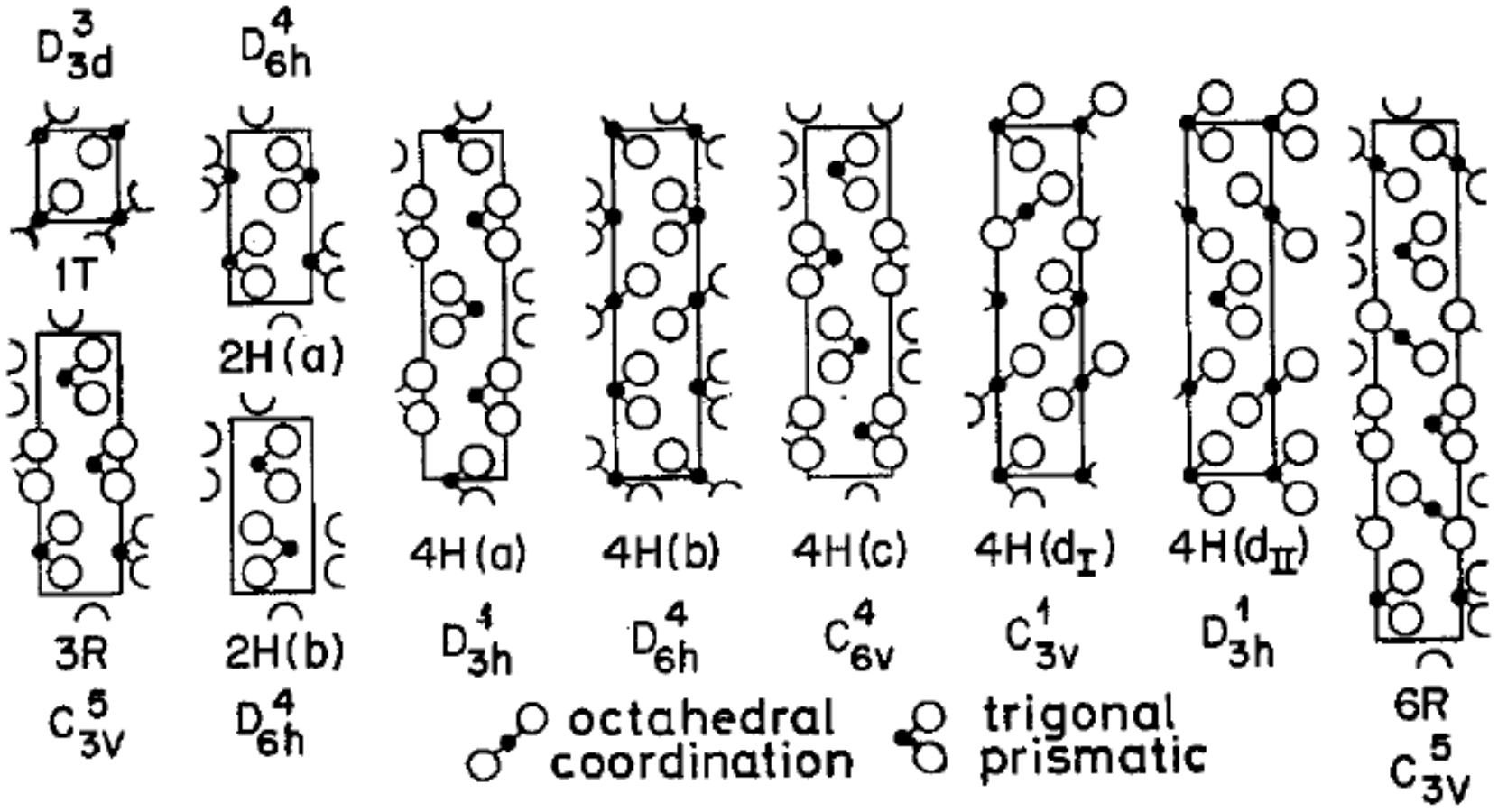
A. Kuc (2015) *Mrs Bulletin*

•DOI:10.1557/MRS.2015.143





CDW in transition metal dichalcogenides



Various polytypes of the layer structure transition metal dichalcogenides

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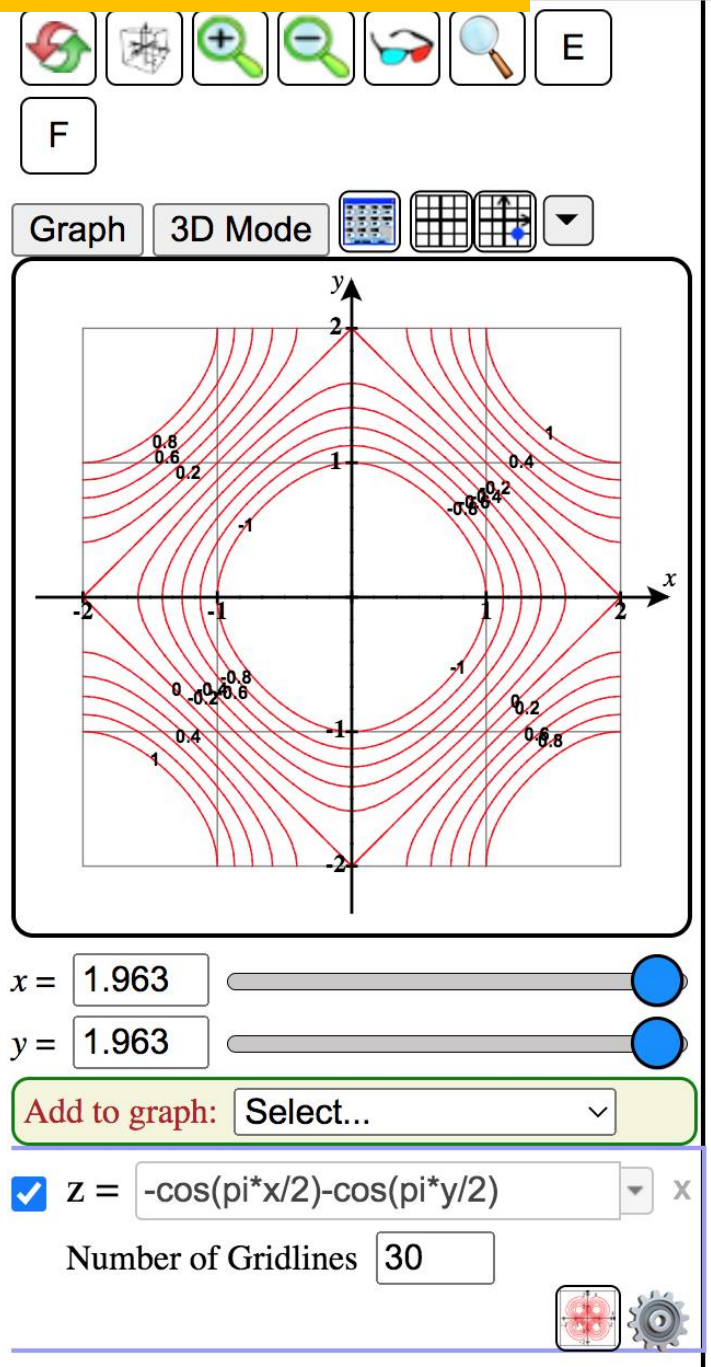
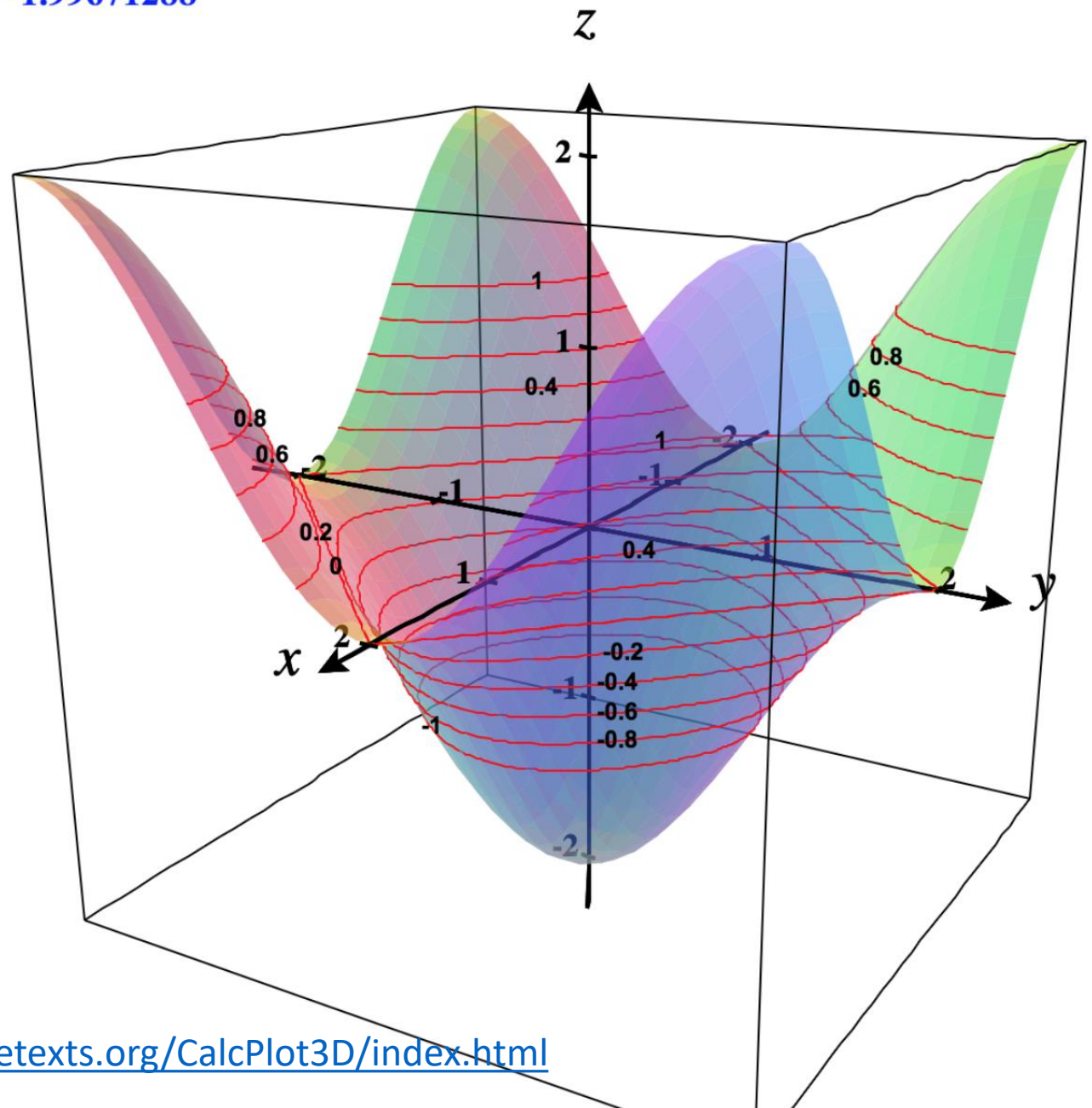
https://doi.org/10.1080/00018736900101307

З попередньої лекції...

Developed with support from NSF-IUSE #1524968.



$f(1.9635, 1.9635) = 1.99671288$



https://c3d.libretexts.org/CalcPlot3D/index.html

З попередньої лекції...

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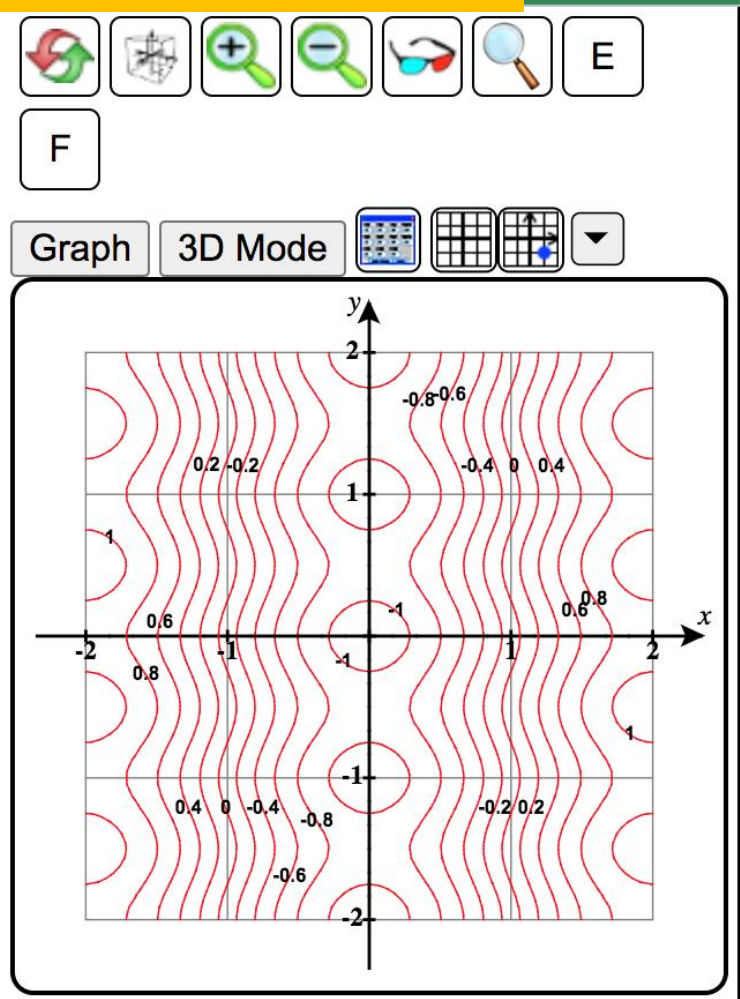

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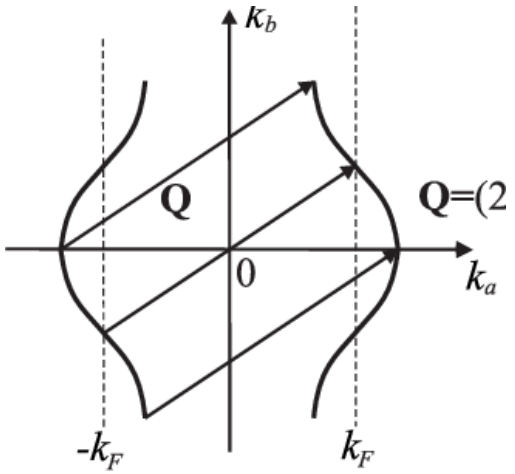

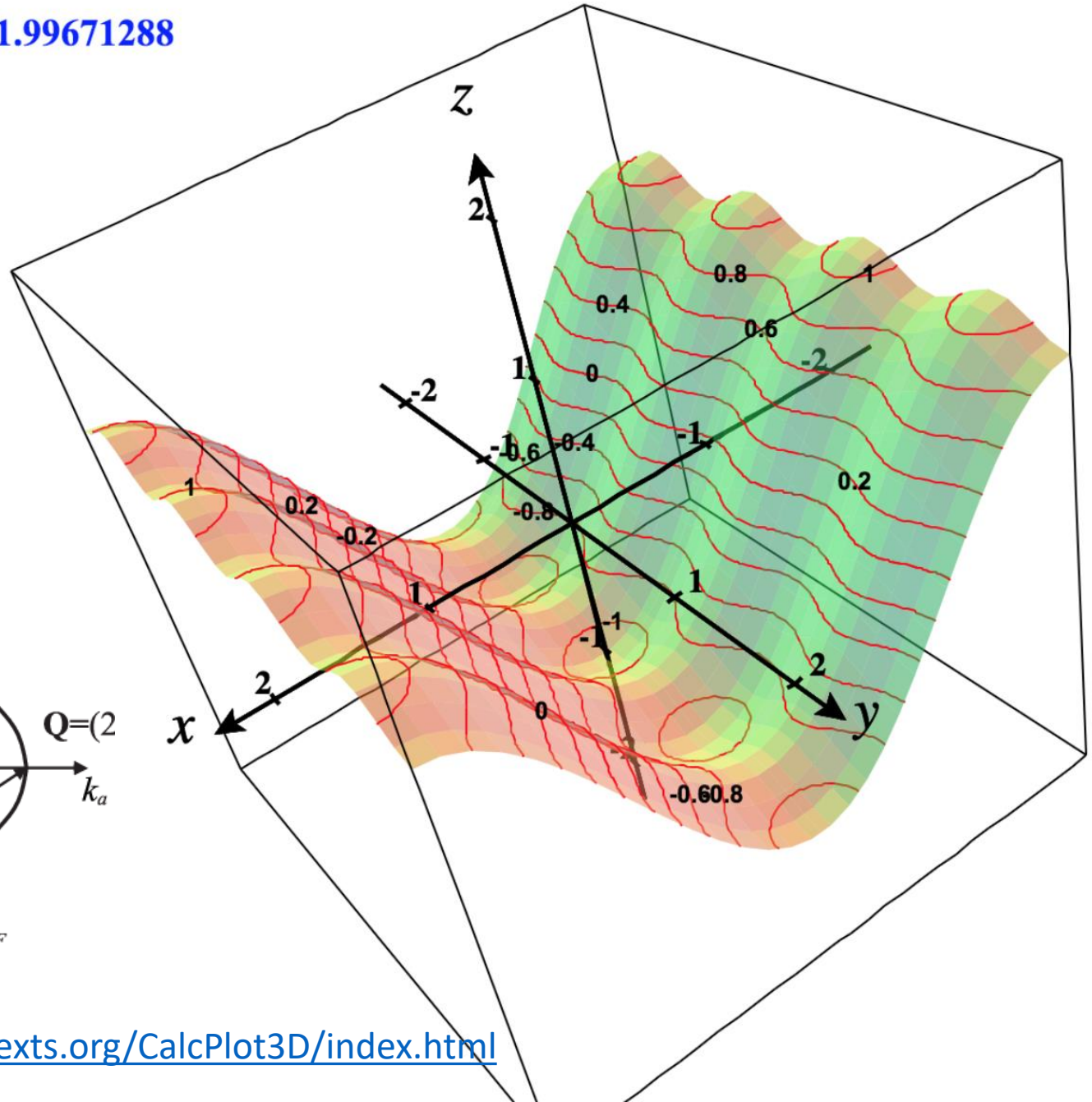

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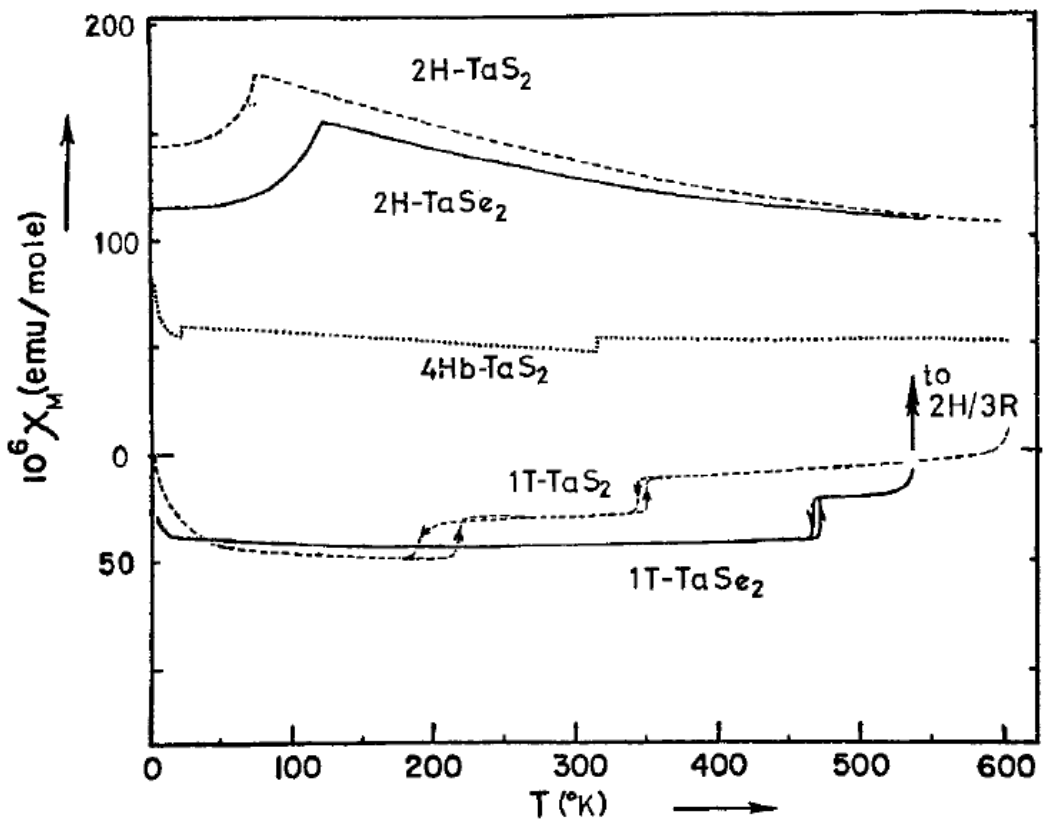
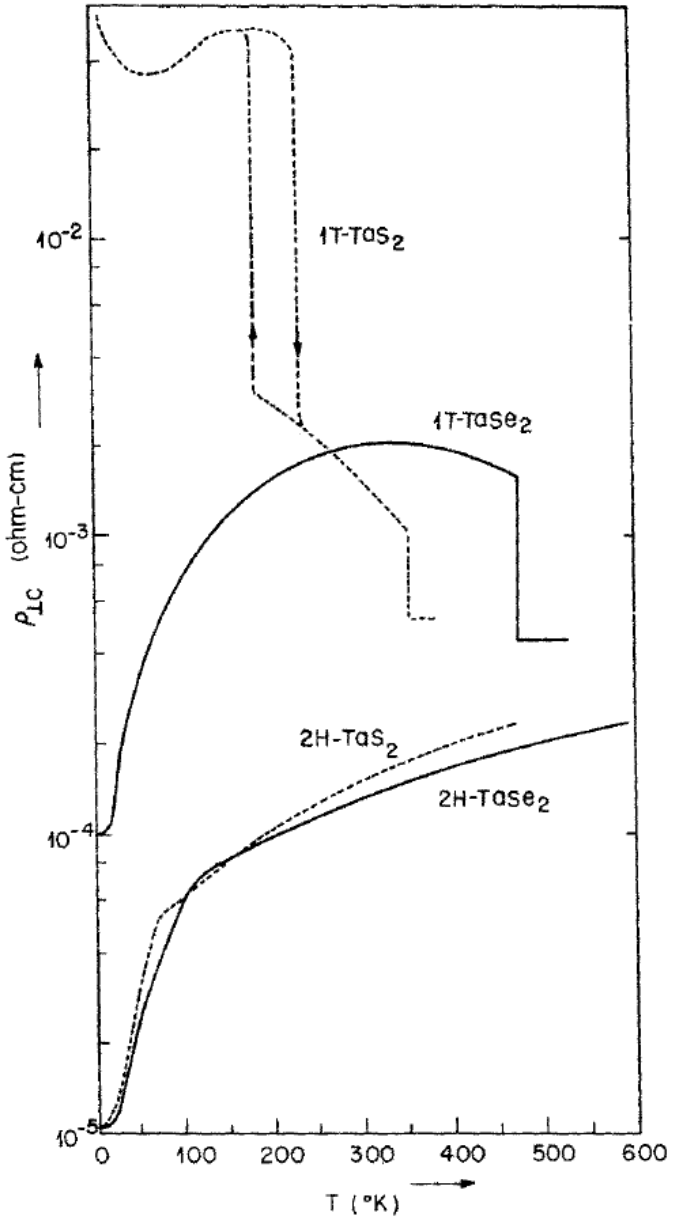
CDW in transition metal dichalcogenides

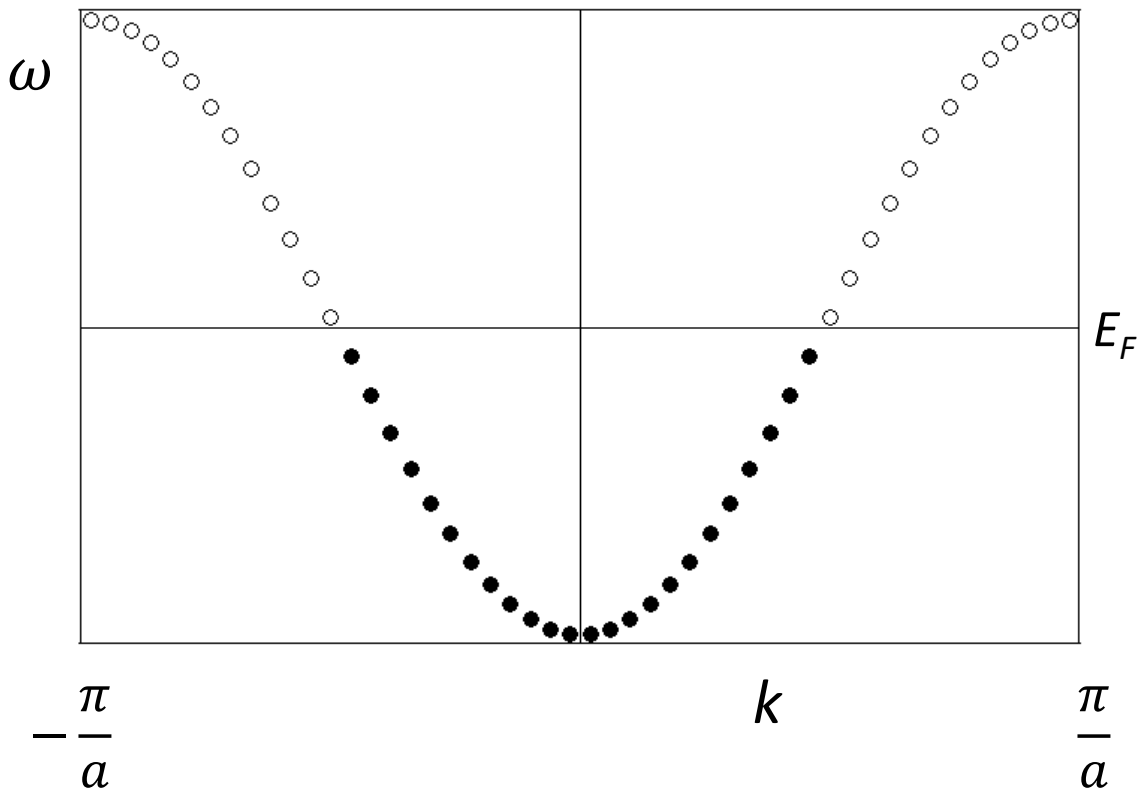


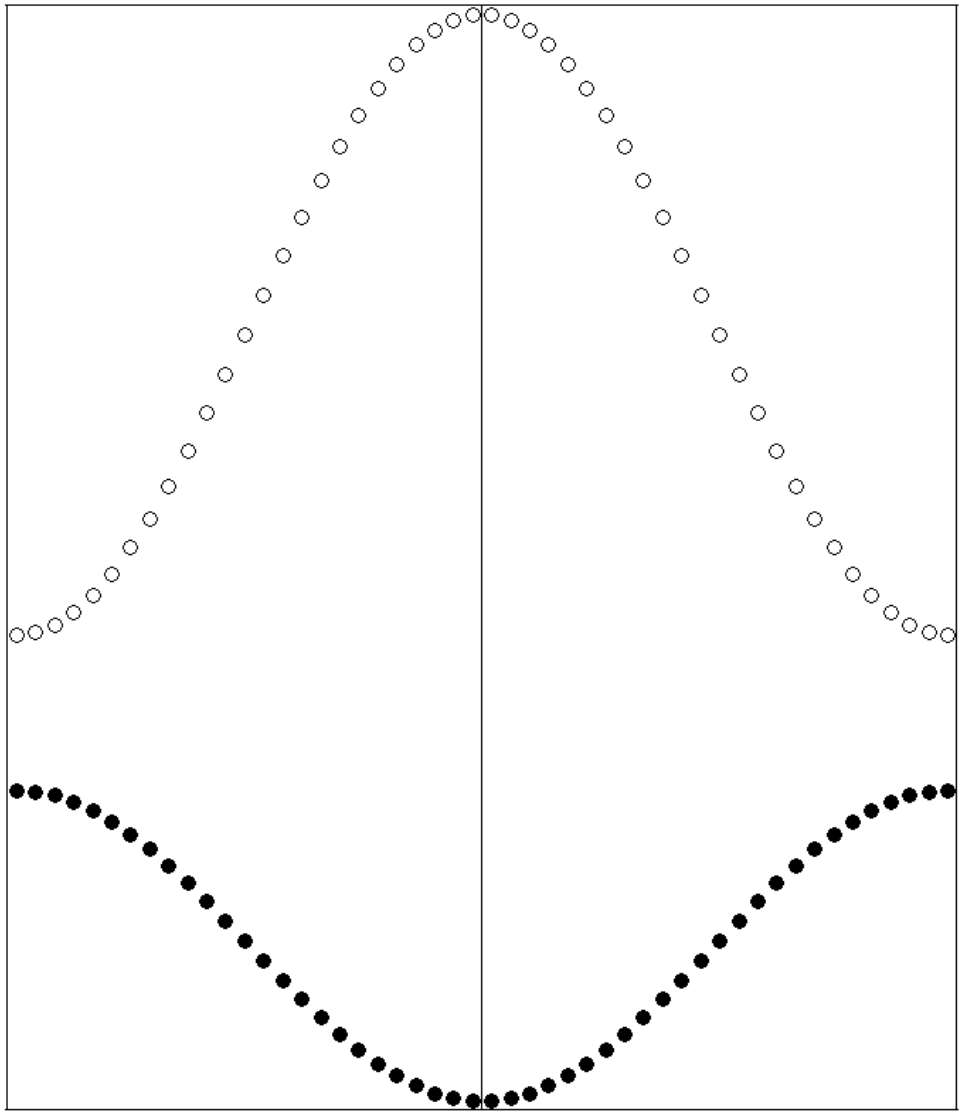
Molar susceptibilities versus T of a variety of tantalum dichaleogenides.



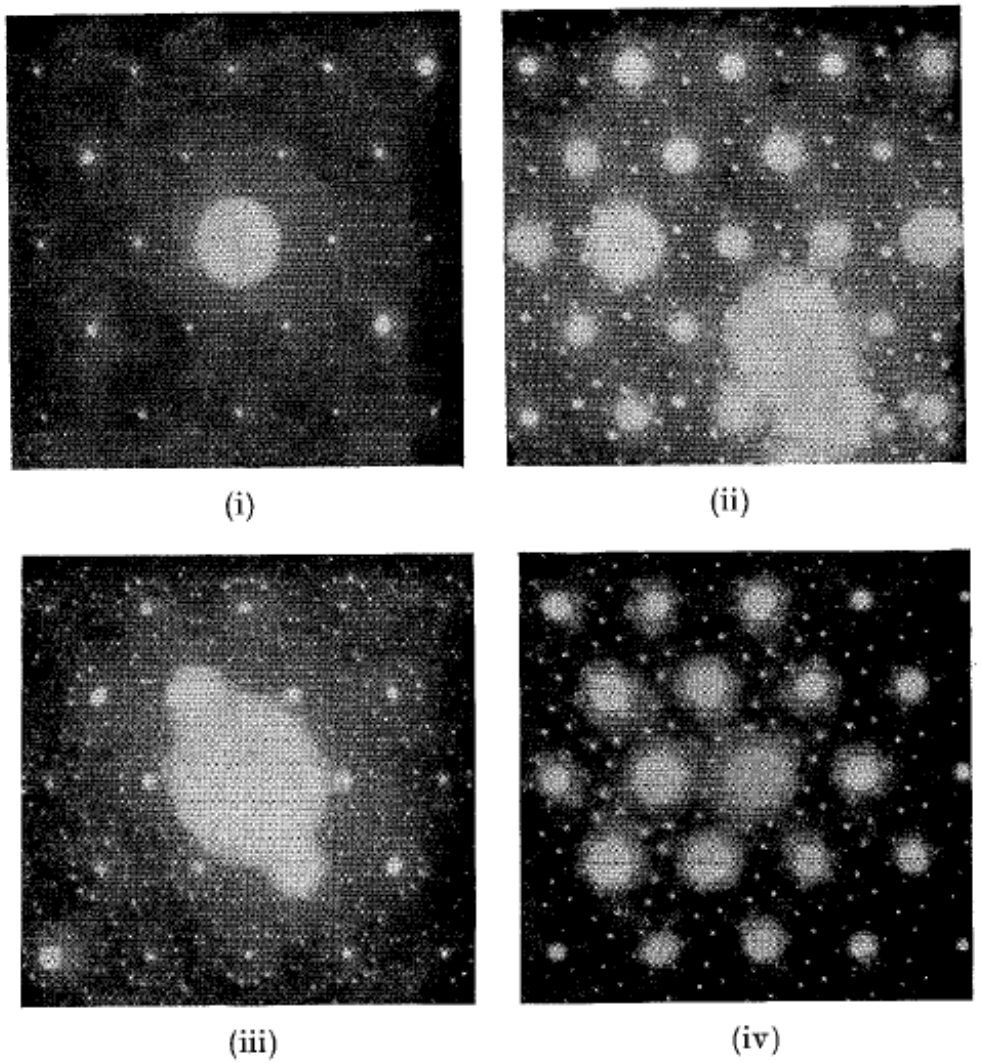
J. A. Wilson et al. Advances in Physics, 24, 117-201 (1975)

Metal *vs* Insulator





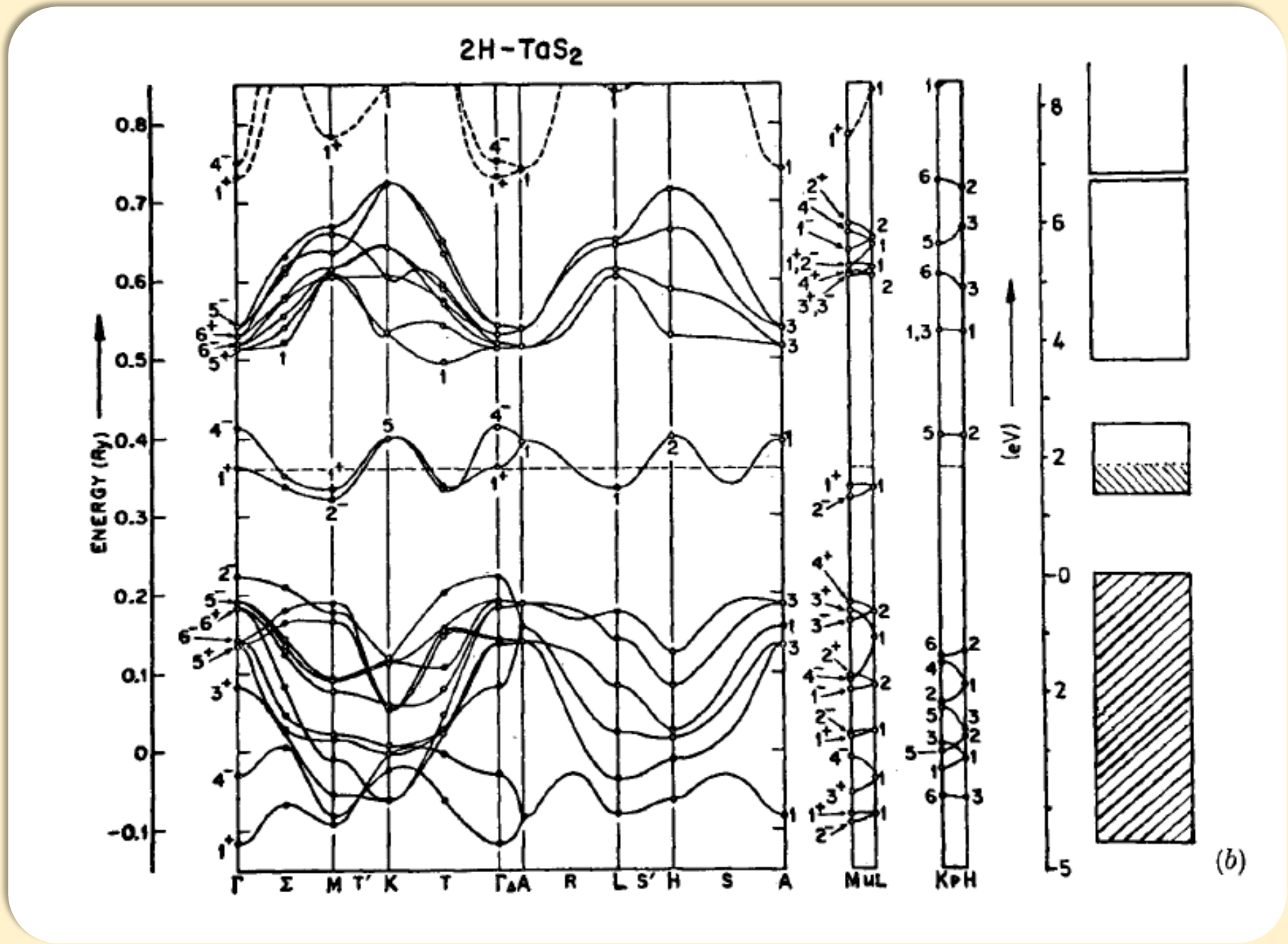
CDW in transition metal dichalcogenides



Electron diffraction plates showing superlattice formation.
(i) 2H-TaS% (300°K).
A crystal showing standard a o parameter.
(ii) 1T-TaS% (300°K). Pattern, for well-oriented sample, from ~/(13) superlattice.
(iii)
4Hb-TaS2 (300°K). Pattern indexable on 13 superlattice. Equivalent to superposifion of ~ and /~-domain patterns.
(iv) 1T-TaS~ (300°K). Basically ~/(13)a o superlattice pattern (here of ~-dolnain type), but with complex 'decoration'.

J. A. Wilson et al. Advances in Physics, 24, 117-201 (1975)

J. A. Wilson et al. Advances in Physics, 24, 117-201 (1975)



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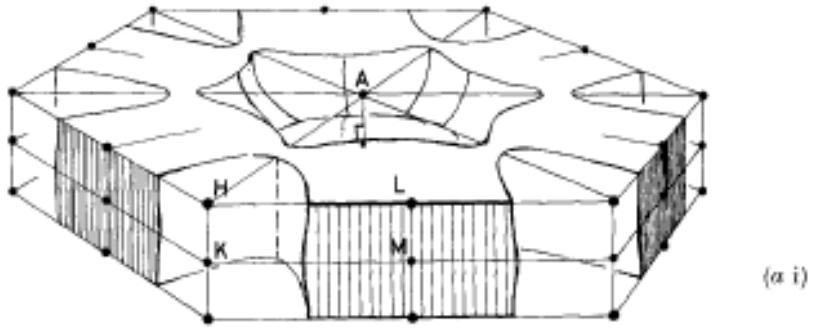
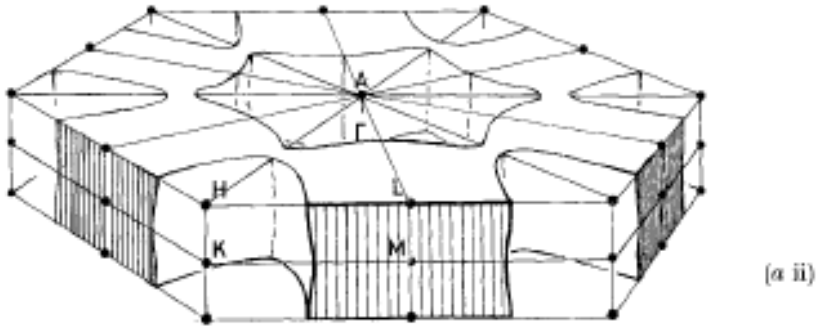


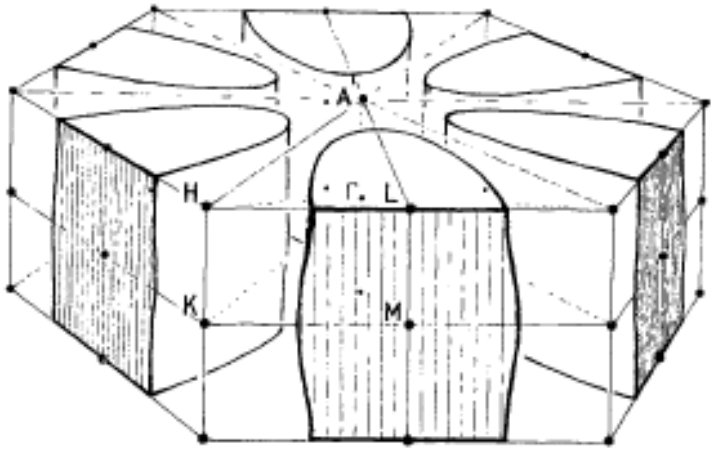
(a i)

2H-TaS_2 lower band



(a ii)

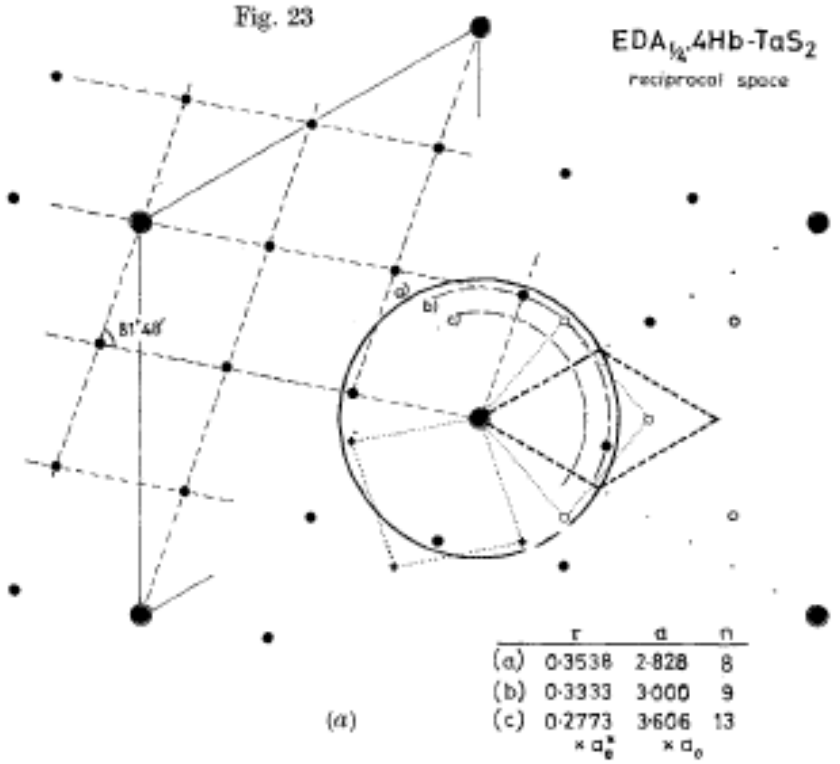
2H-TaS_2 upper band



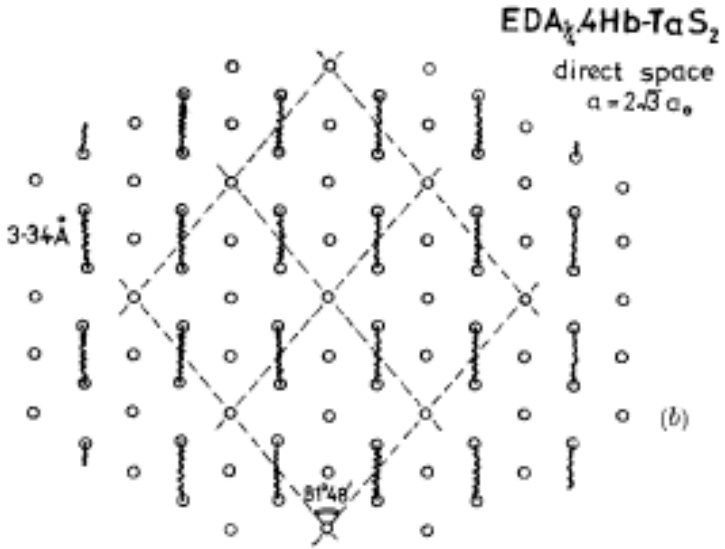
(b)

1T-TaS_2

Fig. 23

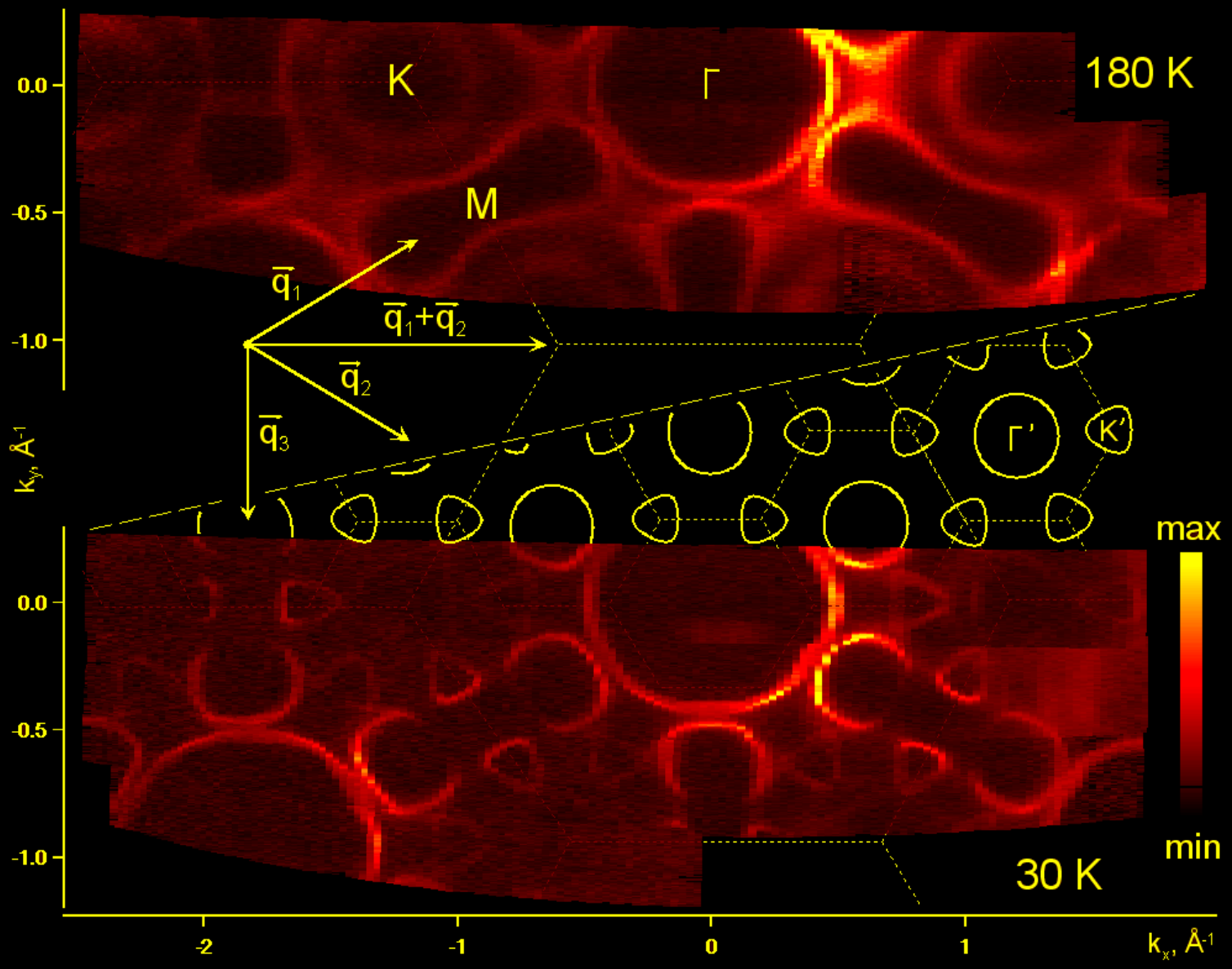


(a)



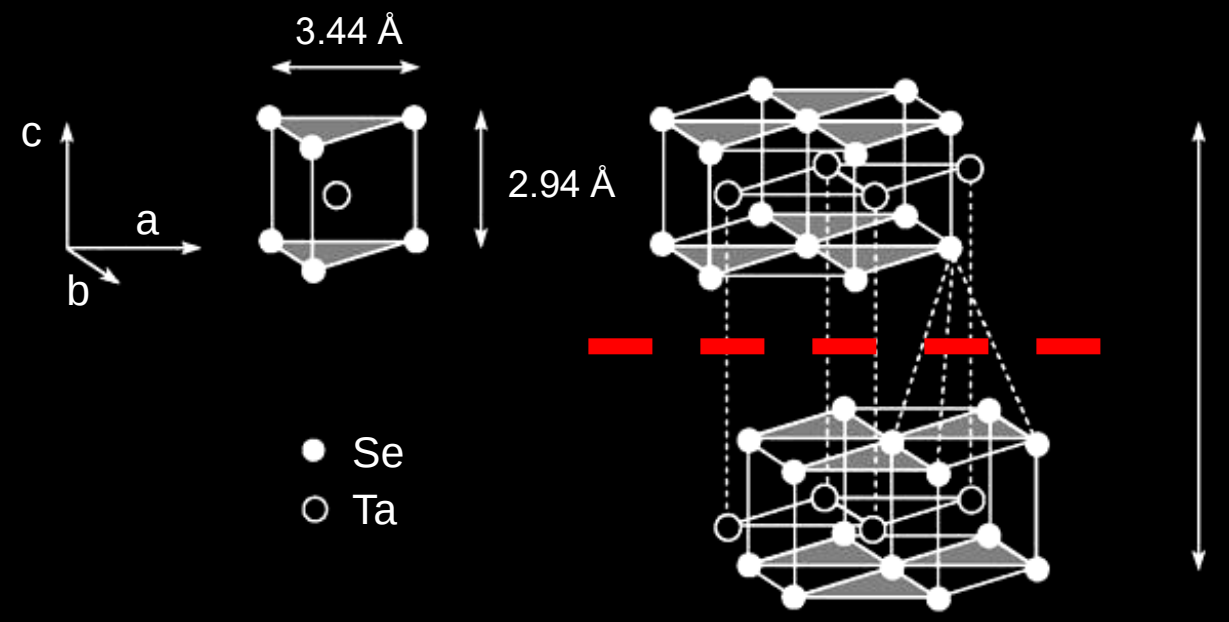
(b)

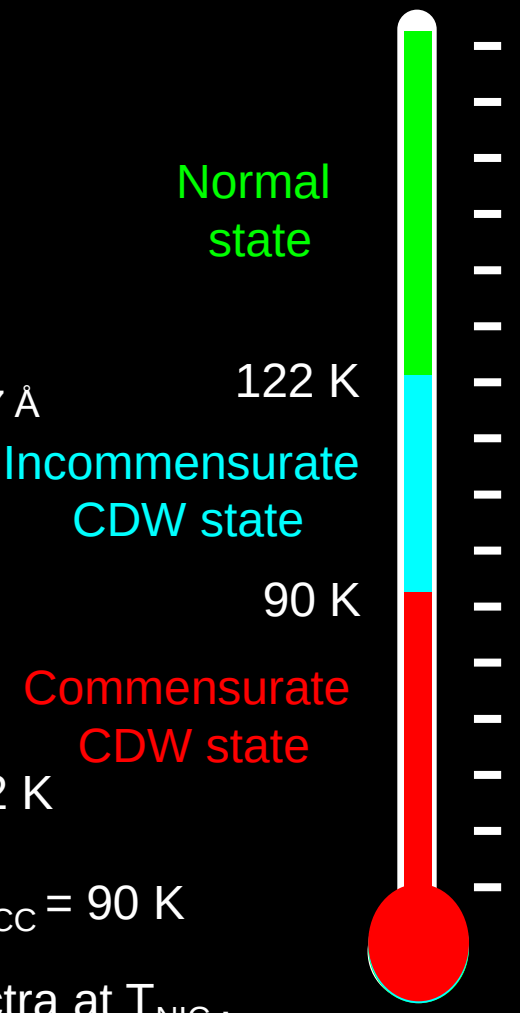
CDW in $TaSe_2$: commensurate CDW state



Borisenko *PRL* 2008

2H-$TaSe_2$ crystal structure, CDW transitions

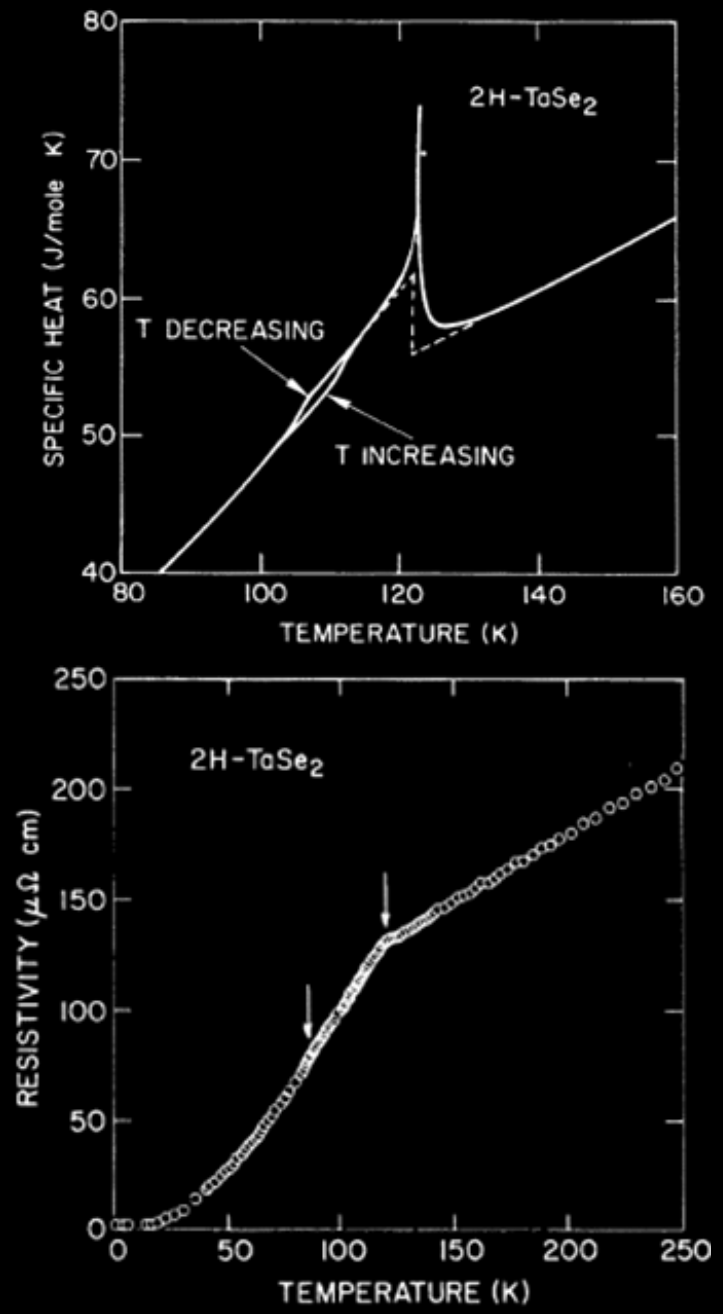


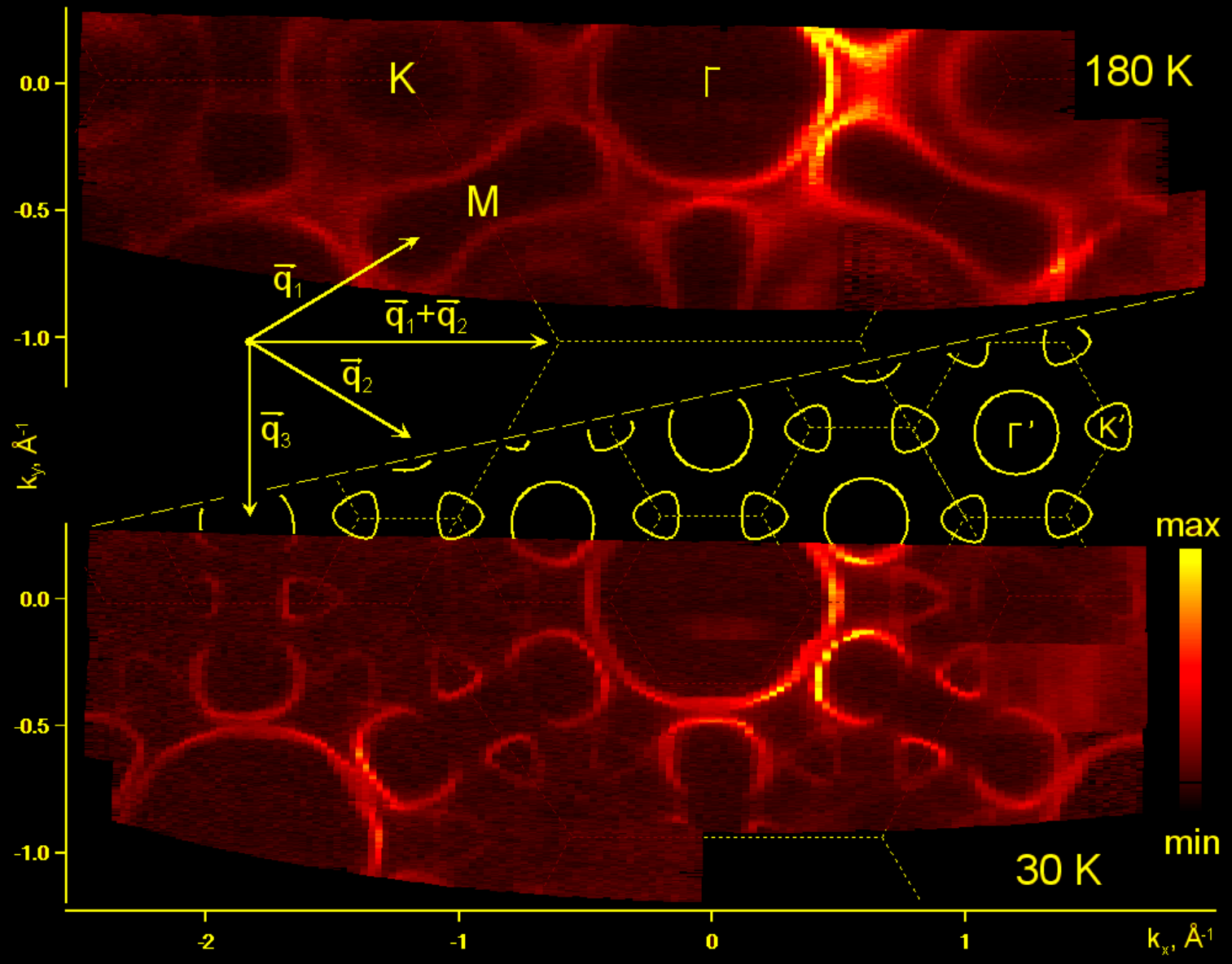


- 2nd-order transition to an incommensurate CDW at T_{NIC} = 122 K
- 1st-order lock-in transition to a 3x3 commensurate CDW at T_{ICC} = 90 K
- What was strange? No nesting. No change in ARPES spectra at T_{NIC} .
  Gap of 24-250 meV only below 90K.

Borisenko 2008

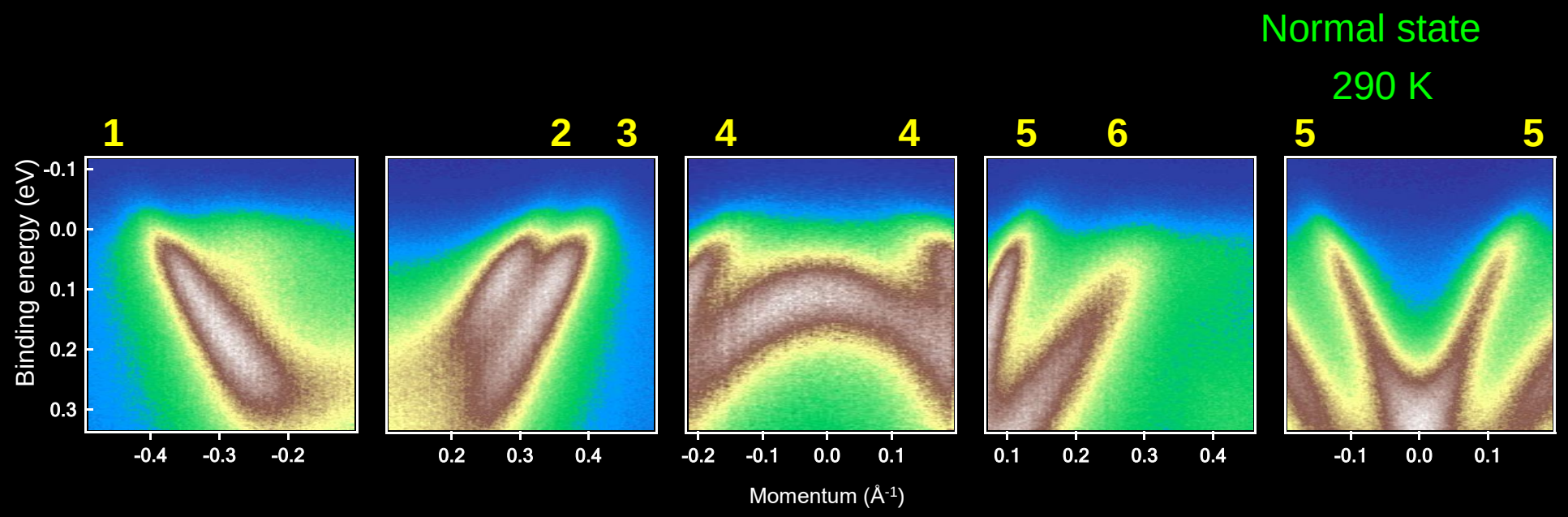
CDW in $TaSe_2$: commensurate CDW state

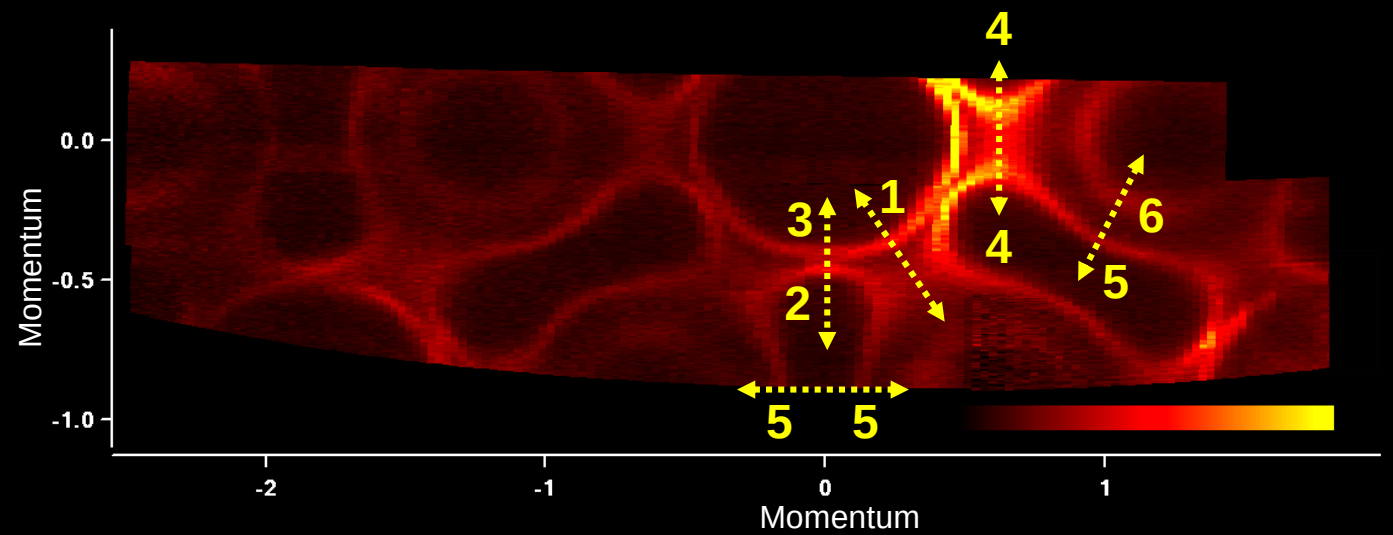




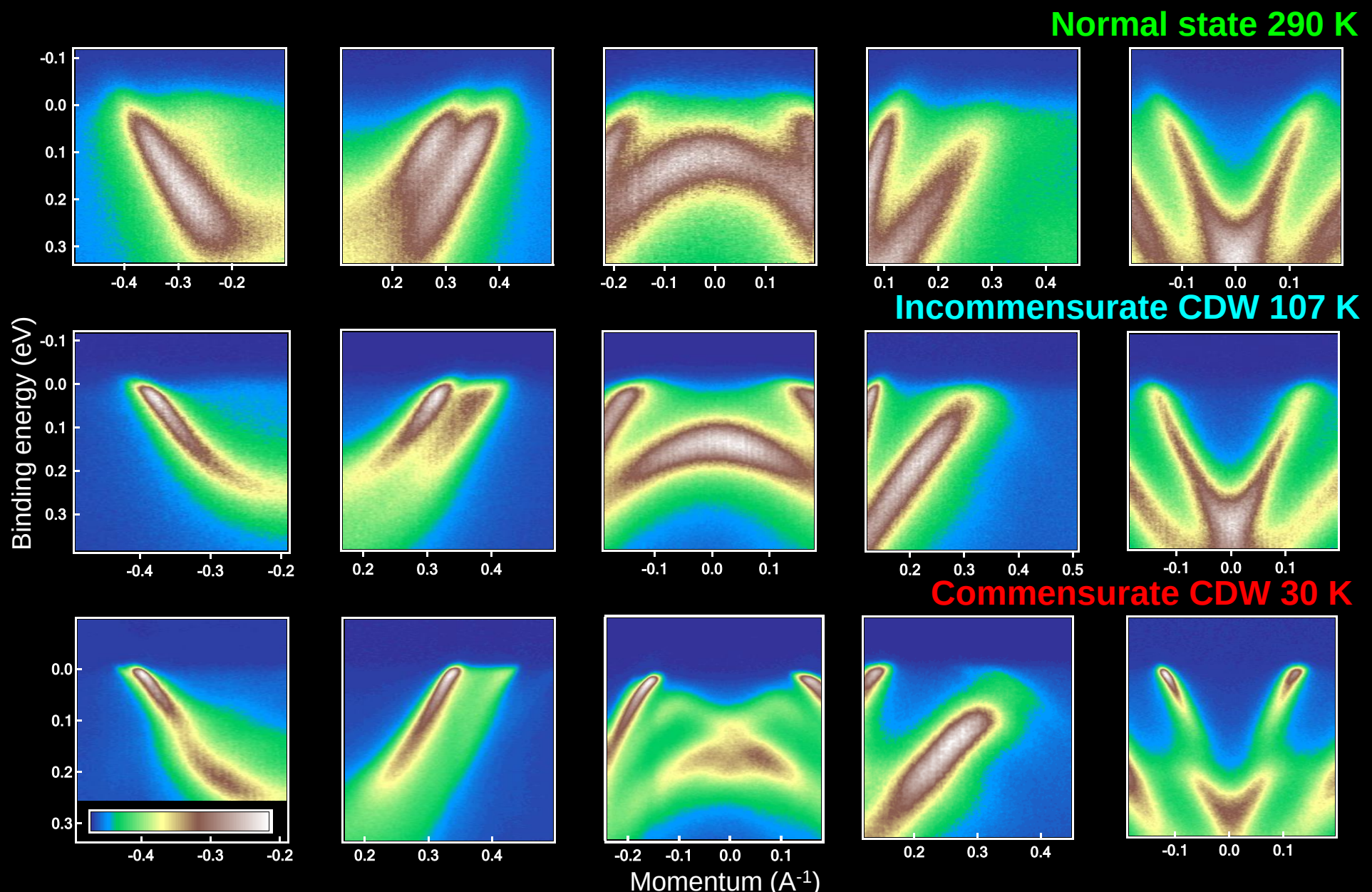
Borisenko *PRL* 2008

Normal state of 2H-$TaSe_2$

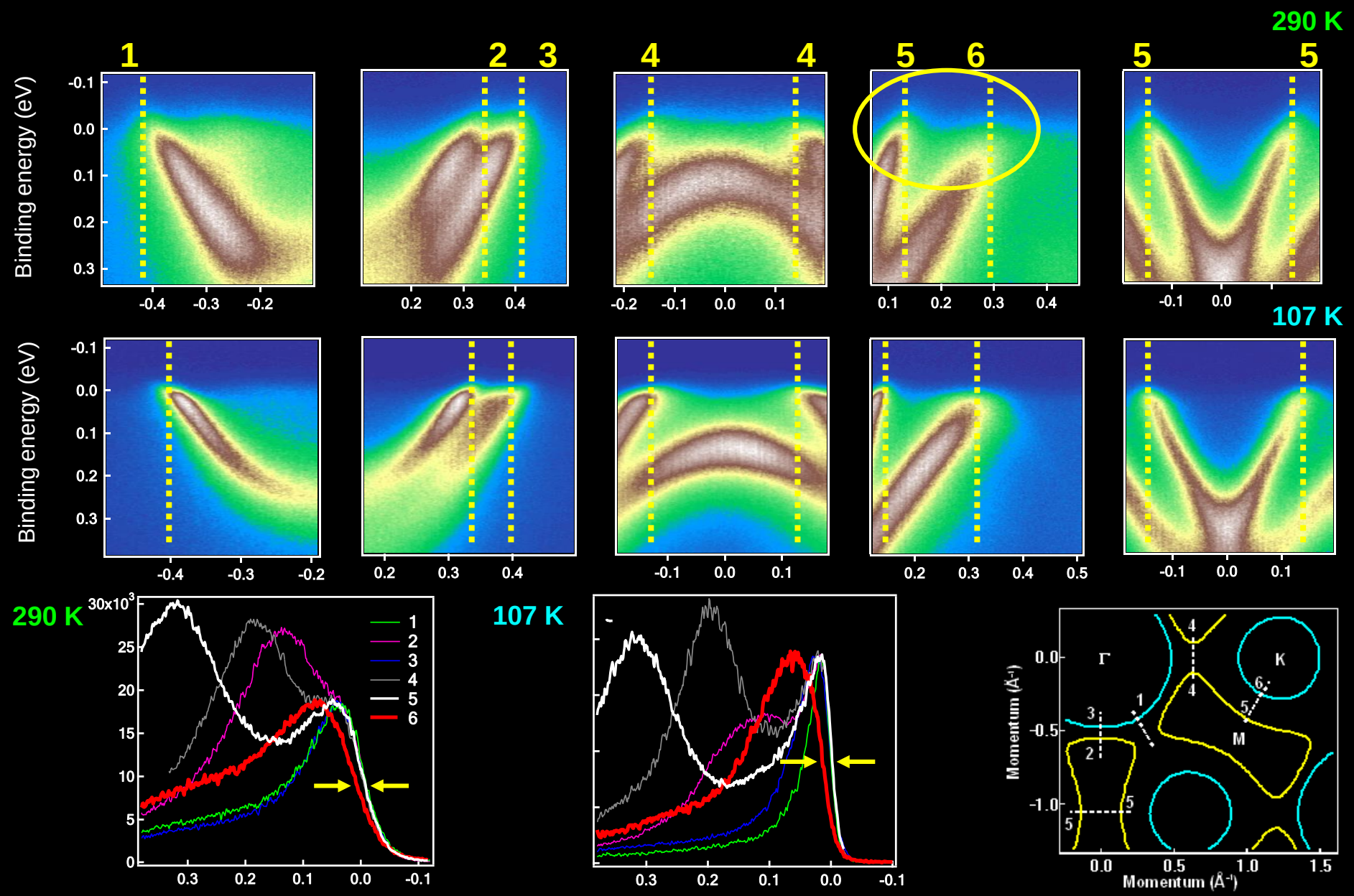




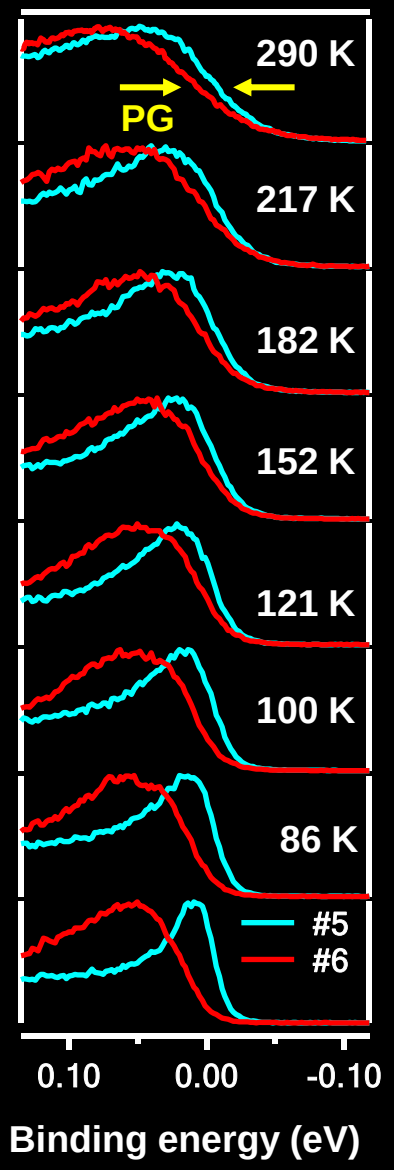
Commensurate CDW state of 2H-$TaSe_2$

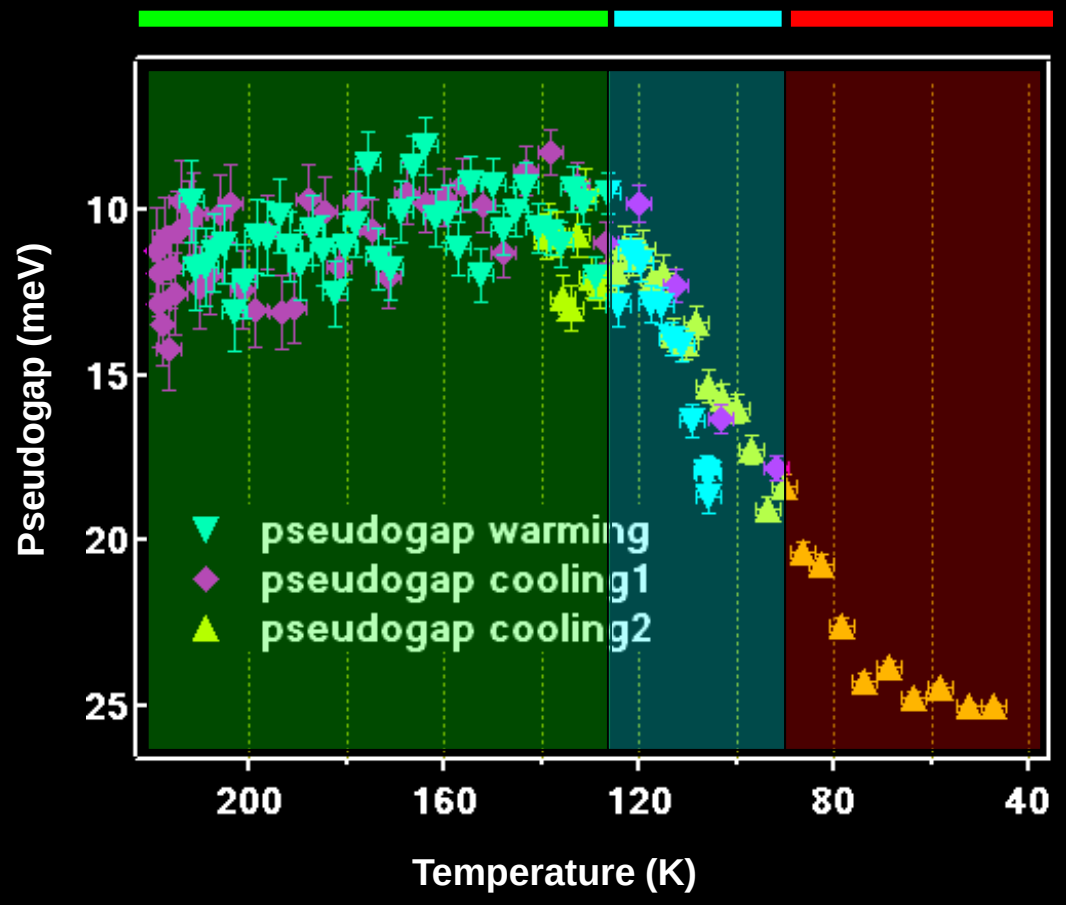


Comparison: IC-CDW and normal state



Pseudogap as a function of temperature

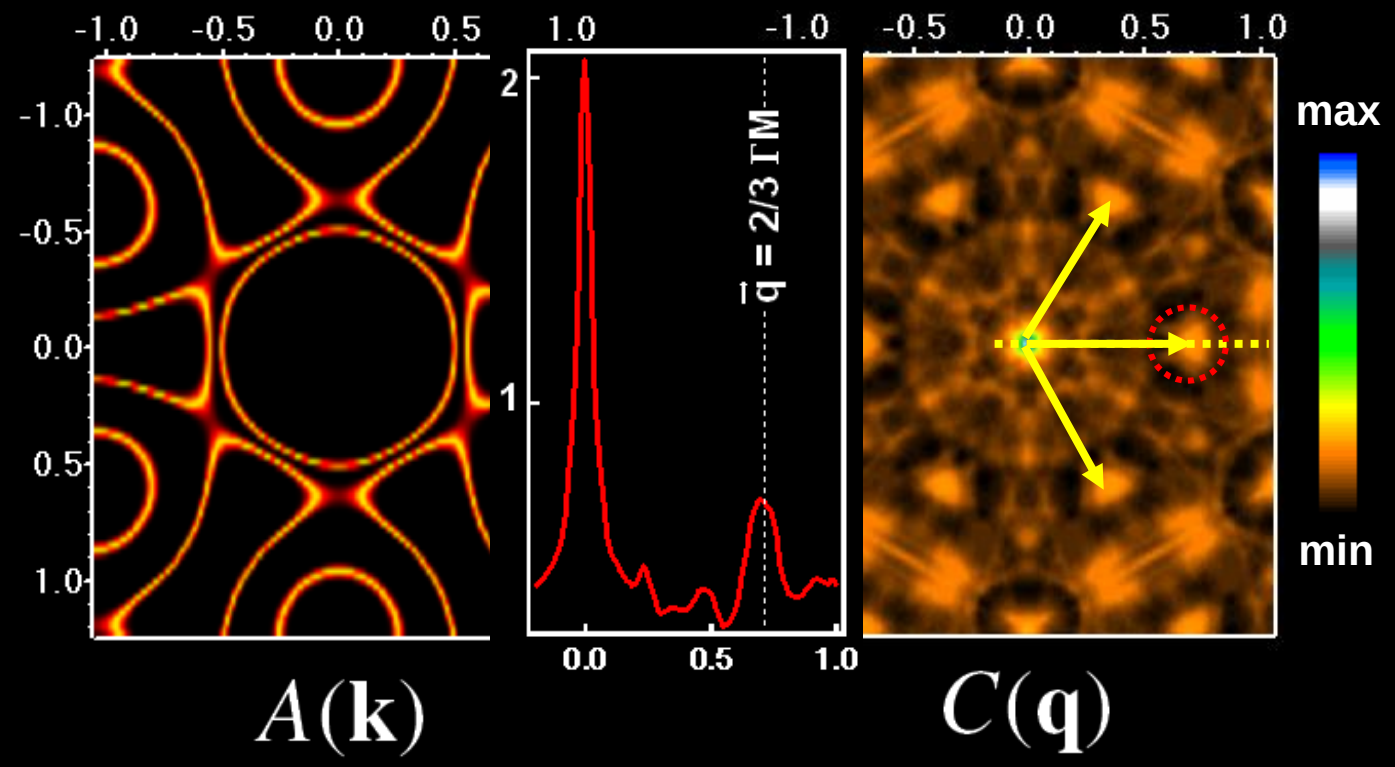




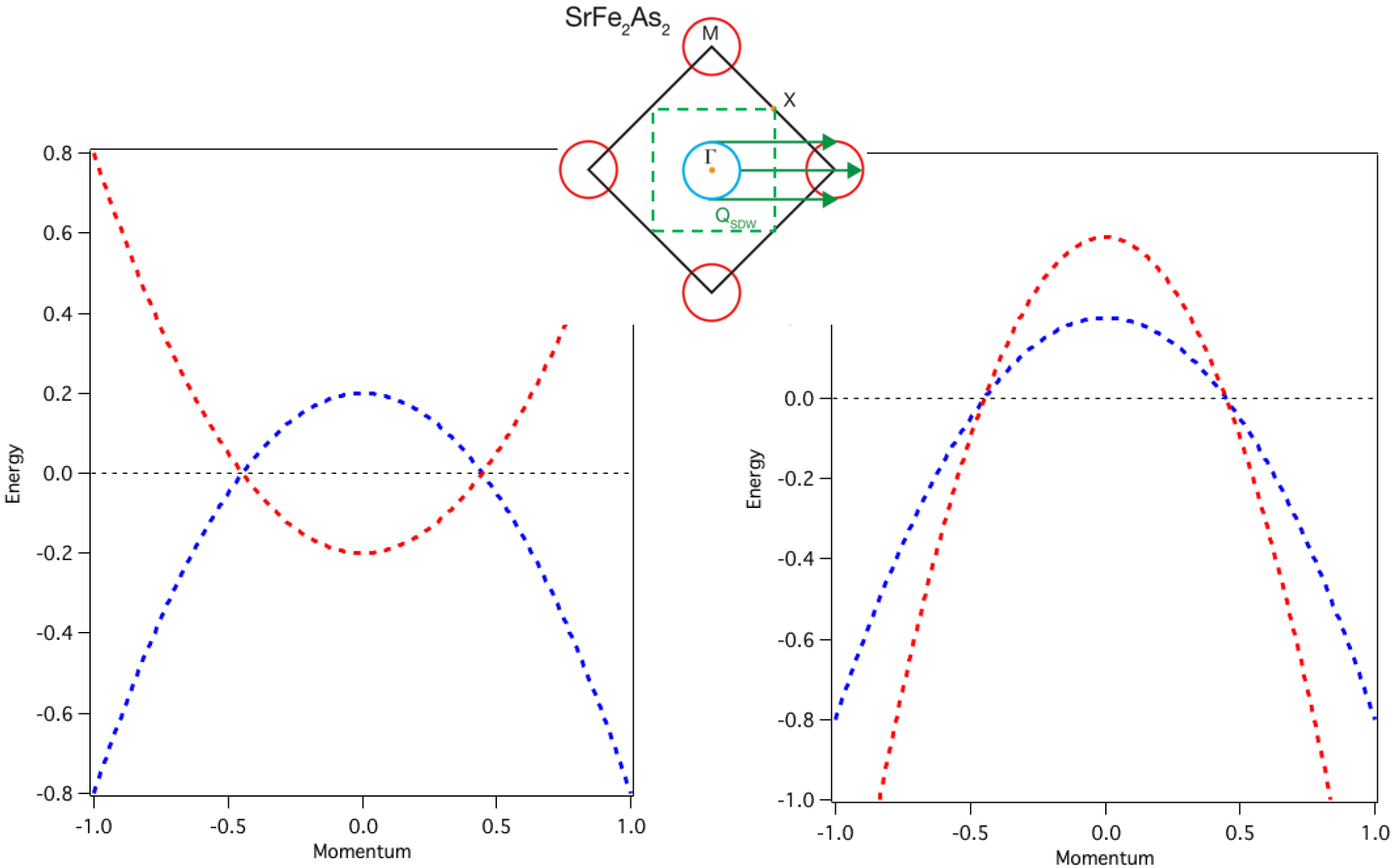
Autocorrelation – measure of nesting

$$\mathbf{AC} \quad A(\mathbf{k}) = \int A(\mathbf{k})A(\mathbf{k}+\mathbf{q})\,\mathrm{d}\mathbf{k} = C(\mathbf{q})$$

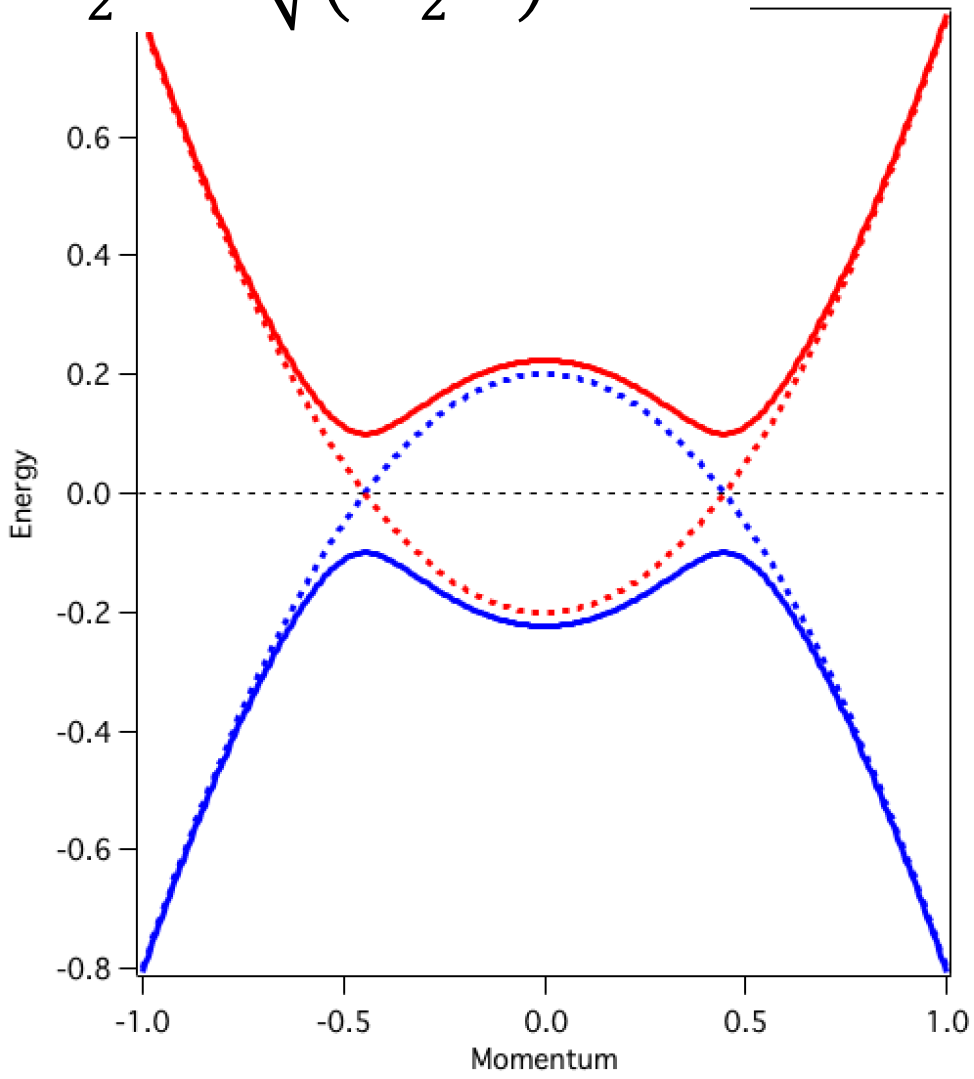
290 K

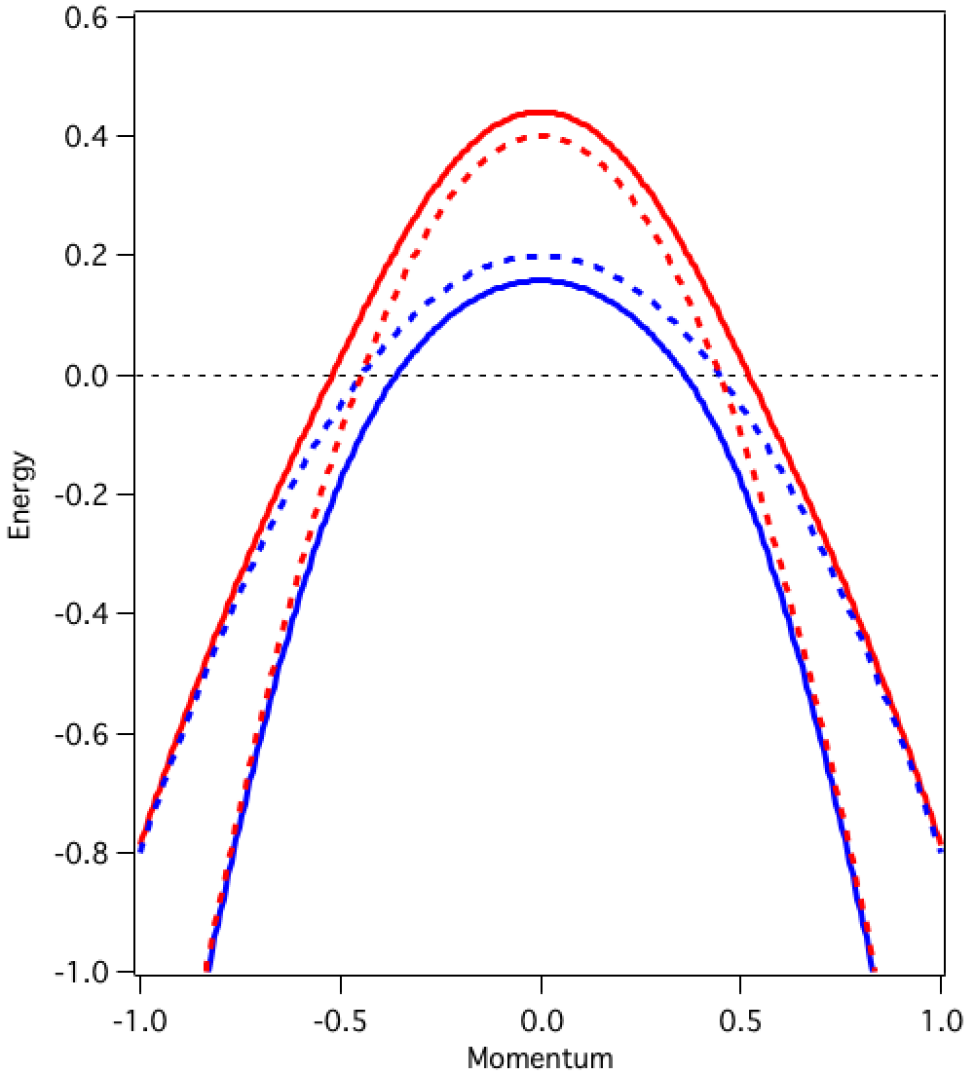


Borisenko *PRL* 2008

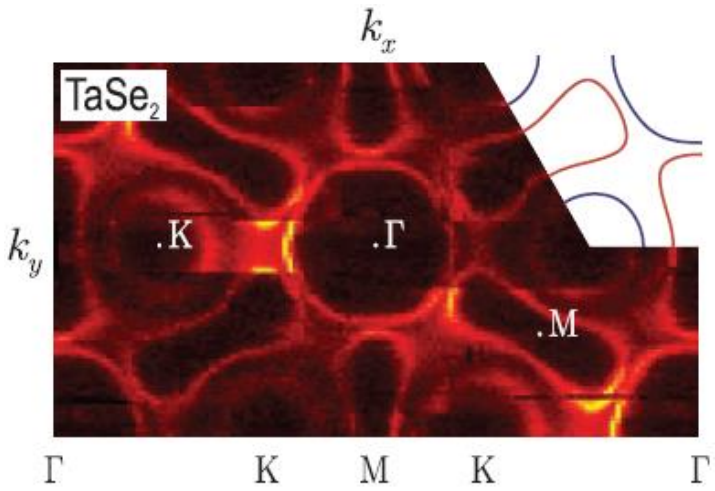

SrFe2As2
M
X
Γ
QSDW
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
-0.8
Energy
-1.0
-0.5
0.0
0.5
1.0
Momentum
0.0
-0.2
-0.4
-0.6
-0.8
-1.0
Energy
-1.0
-0.5
0.0
0.5
1.0
Momentum

$$\varepsilon_{\pm} = \frac{\varepsilon_1+\varepsilon_2}{2} \pm \sqrt{\left(\frac{\varepsilon_1-\varepsilon_2}{2}\right)^2 + \Delta^2}$$



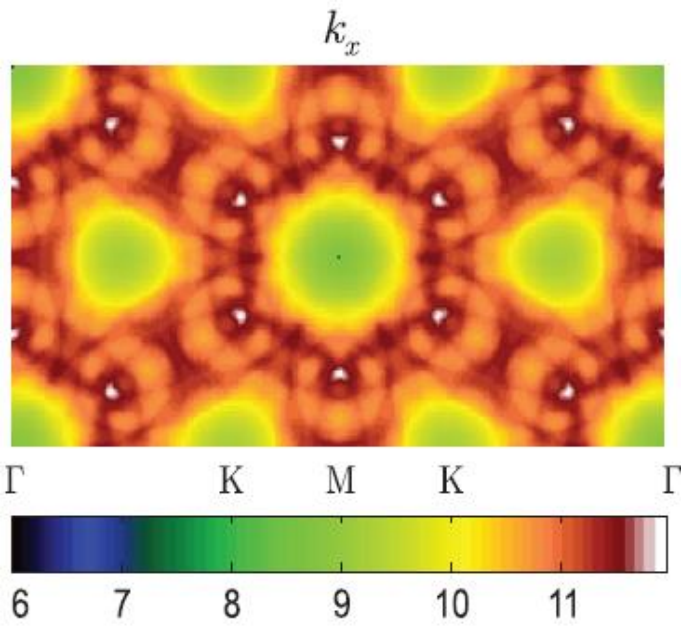


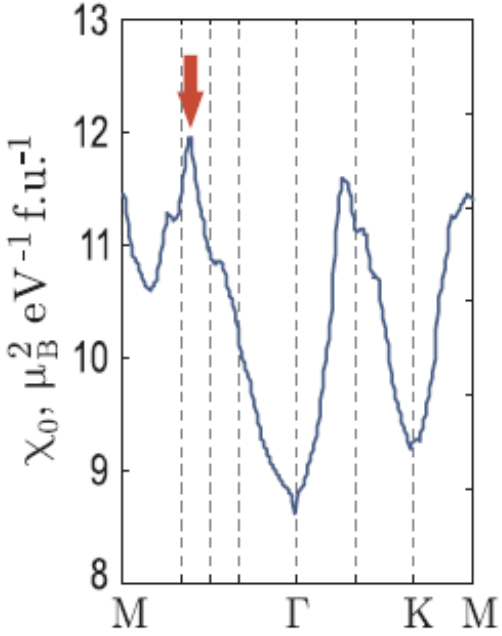
Fermi surface nesting and Lindhard function

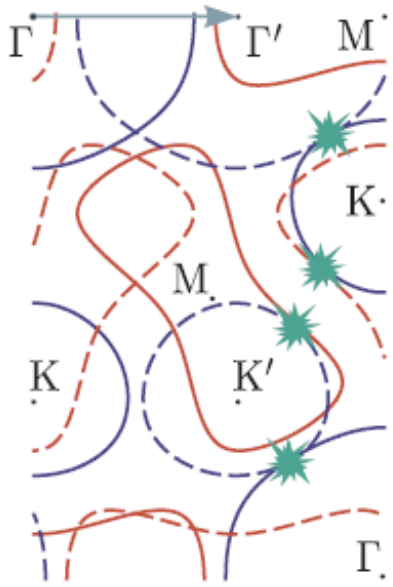


$$\chi_{\mathbf{q}} = \sum_{\mathbf{k}} [n_F(\epsilon_{\mathbf{k}}) - n_F(\epsilon_{\mathbf{k+q}})]/(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k+q}})$$

$$\chi = G \star G$$







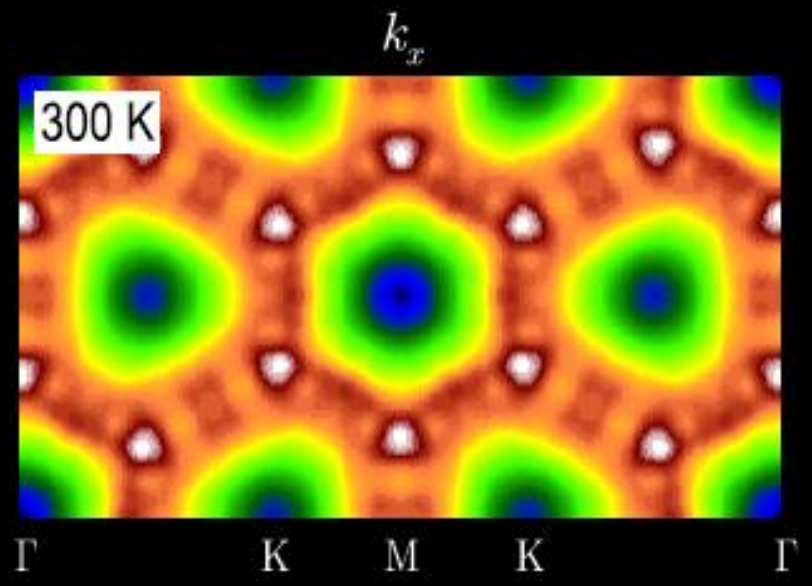
Inosov *NJP* 2008

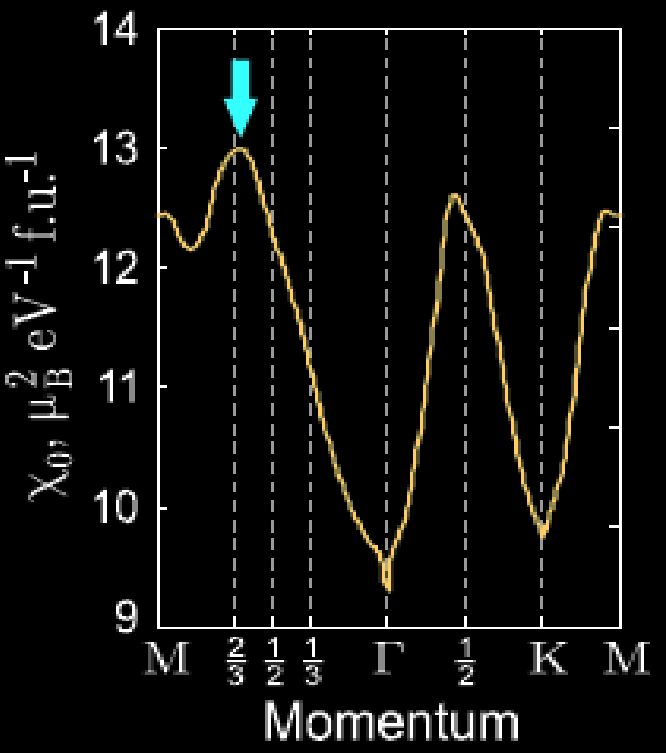
Electron susceptibility

$$\chi_0(\mathbf{q},\omega) = 2\int \frac{d\mathbf{k}}{(2\pi)^d}\,\frac{n_F(\epsilon_{\mathbf{k}}) - n_F(\epsilon_{\mathbf{k}+\mathbf{q}})}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}} + \omega + i0^+}$$

Lindhard functions at $\omega \to 0$

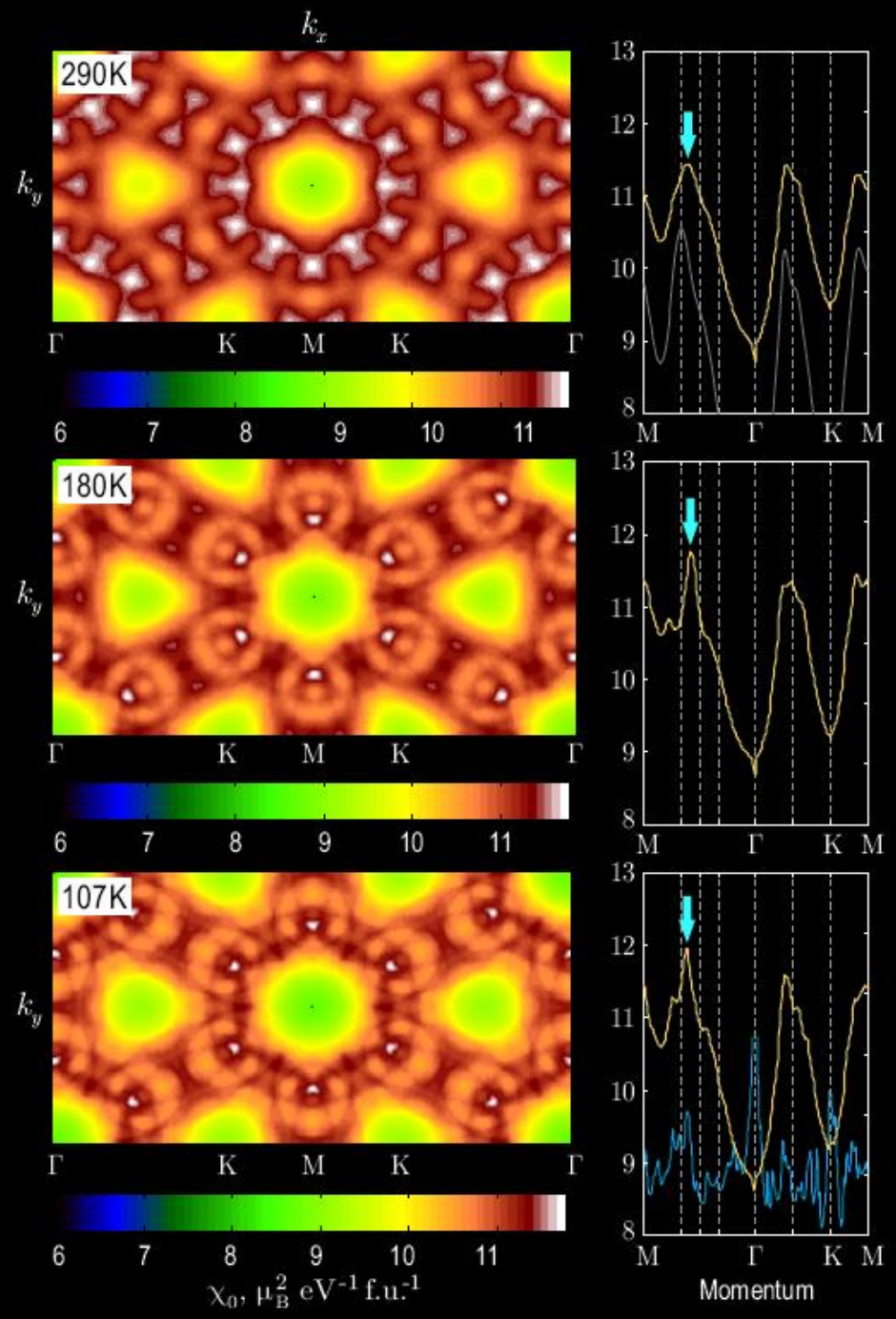
$$\chi_{\mathbf{q}} = \sum_{\mathbf{k}} \frac{n_F(\epsilon^a_{\mathbf{k}}) - n_F(\epsilon^a_{\mathbf{k}+\mathbf{q}})}{\epsilon^a_{\mathbf{k}} - \epsilon^a_{\mathbf{k}+\mathbf{q}}} + \sum_{\mathbf{k}} \frac{n_F(\epsilon^a_{\mathbf{k}}) - n_F(\epsilon^b_{\mathbf{k}+\mathbf{q}})}{\epsilon^a_{\mathbf{k}} - \epsilon^b_{\mathbf{k}+\mathbf{q}}}$$
$$+ \sum_{\mathbf{k}} \frac{n_F(\epsilon^b_{\mathbf{k}}) - n_F(\epsilon^a_{\mathbf{k}+\mathbf{q}})}{\epsilon^b_{\mathbf{k}} - \epsilon^a_{\mathbf{k}+\mathbf{q}}} + \sum_{\mathbf{k}} \frac{n_F(\epsilon^b_{\mathbf{k}}) - n_F(\epsilon^b_{\mathbf{k}+\mathbf{q}})}{\epsilon^b_{\mathbf{k}} - \epsilon^b_{\mathbf{k}+\mathbf{q}}}$$

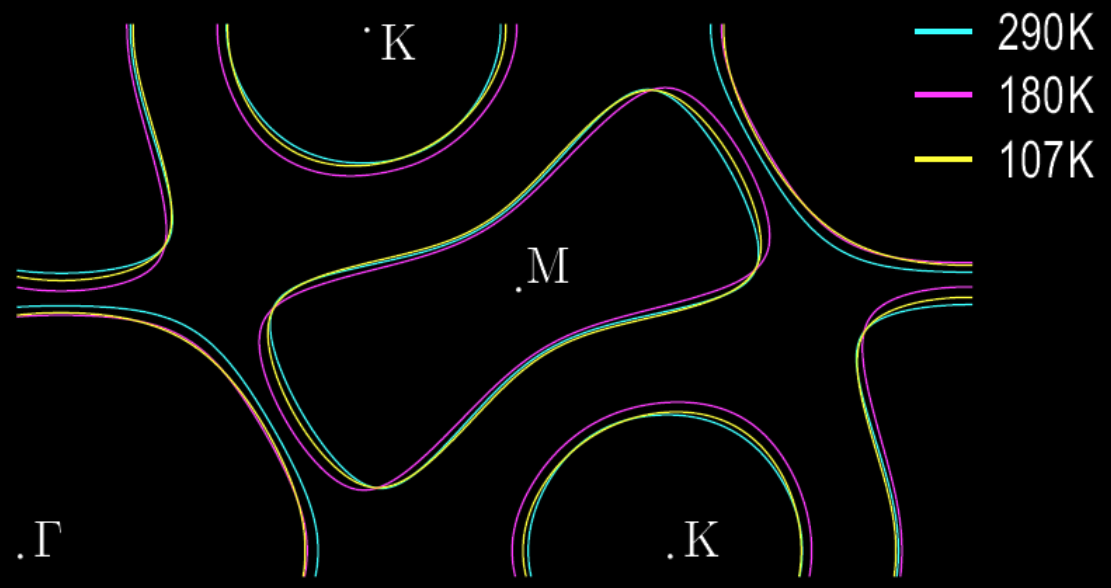




Inosov arXiv:0805.4105, arXiv:0807.3929

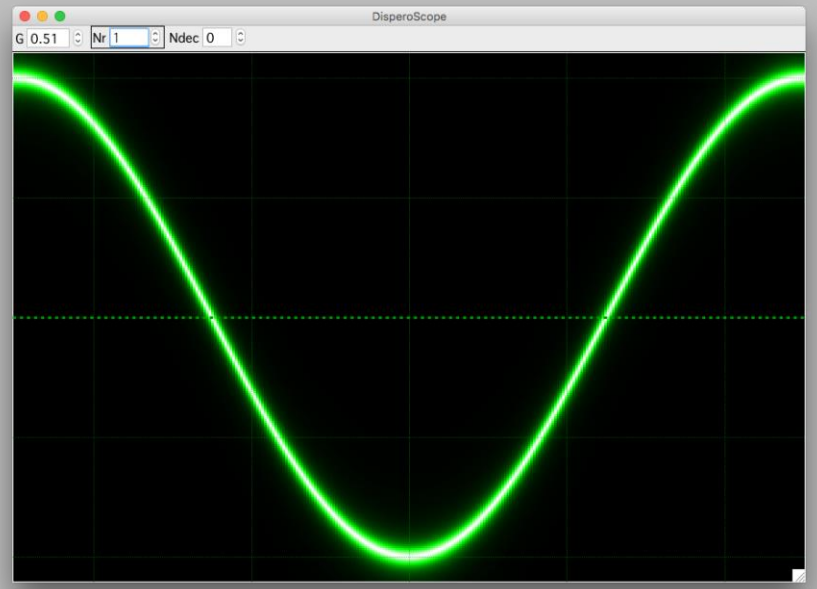
Temperatuire variations

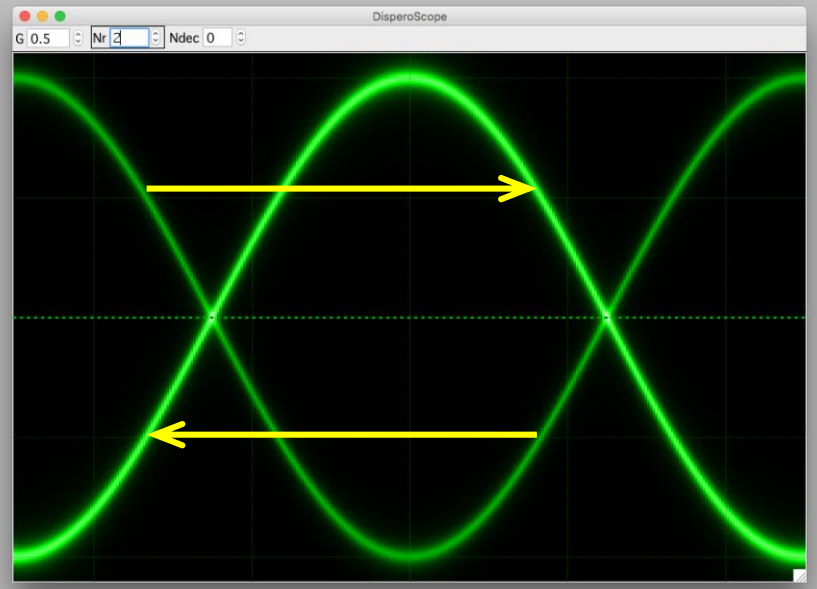


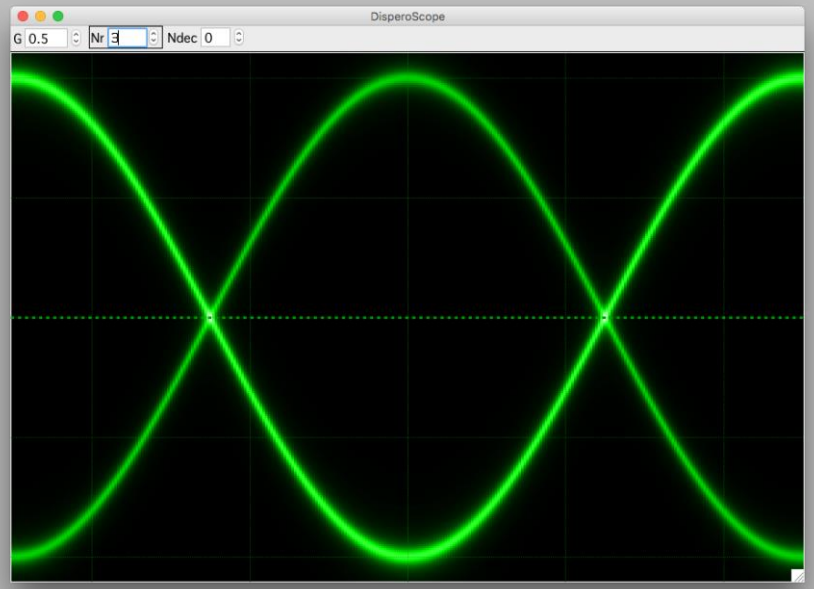


Inosov arXiv:0805.4105, arXiv:0807.3929

Commensurate *vs* Incommensurate

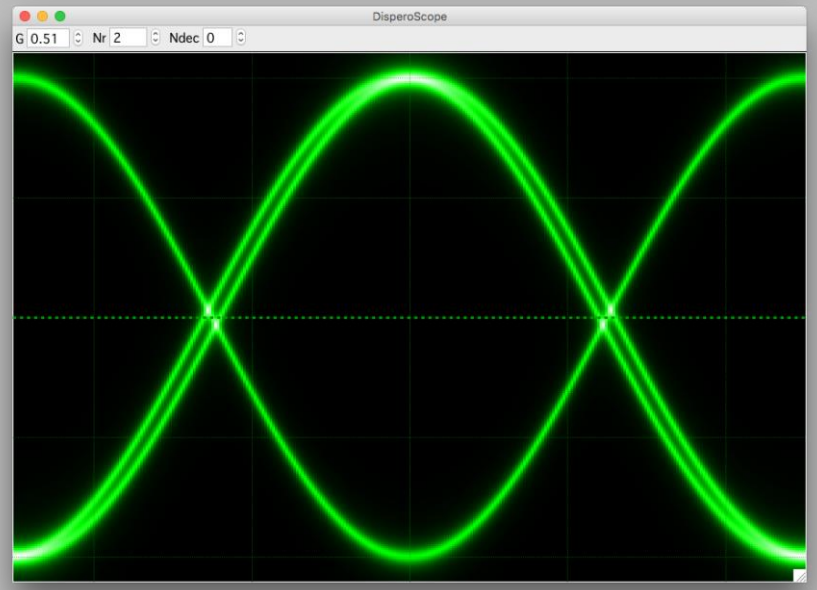


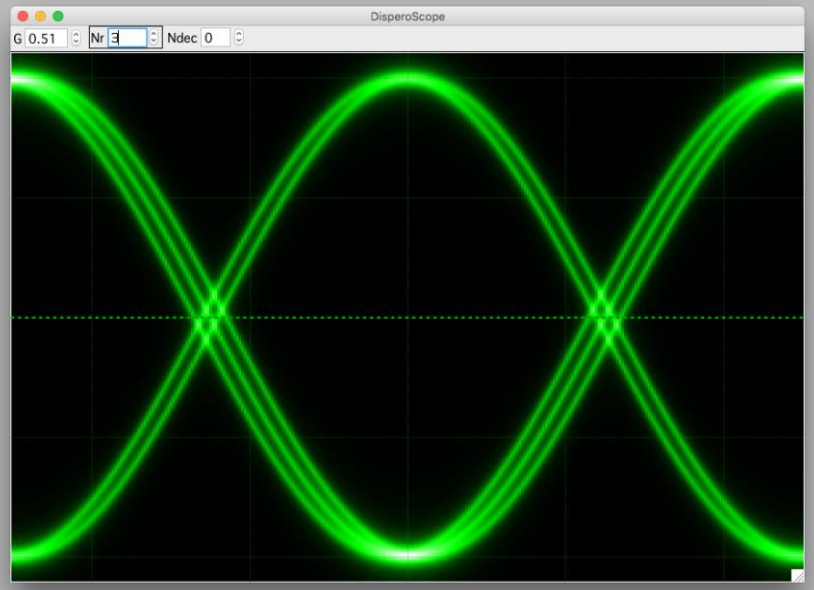




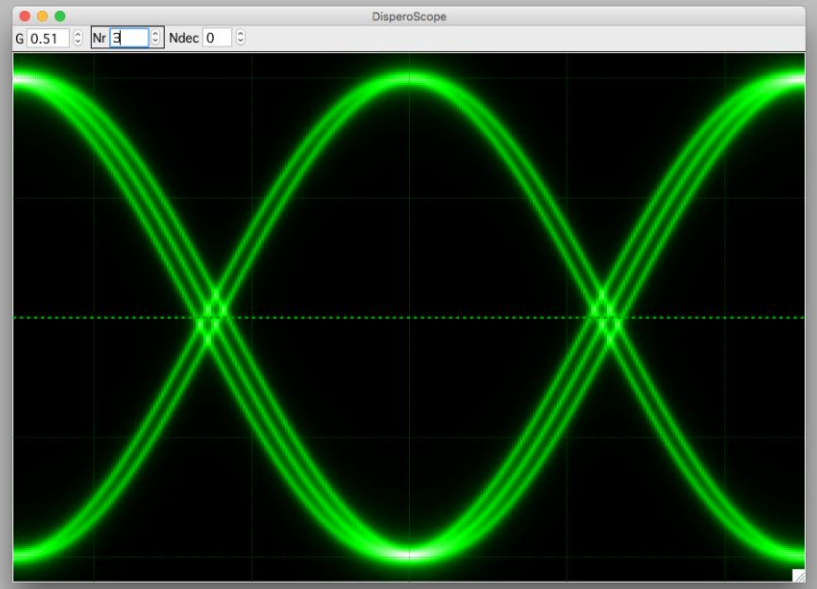
$$A(k,\omega) = \\ = \sum_{i=-(Nr-1)}^{Nr-1} \frac{1}{(\omega - \varepsilon_i(k))^2 + \delta^2}$$

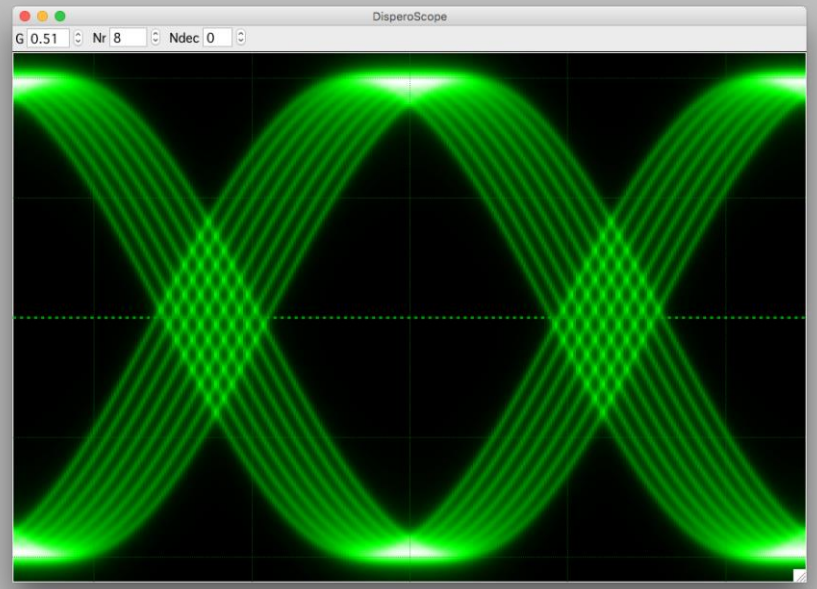
$$\varepsilon_i(k) = -\cos[2\pi(x + Gi)]$$

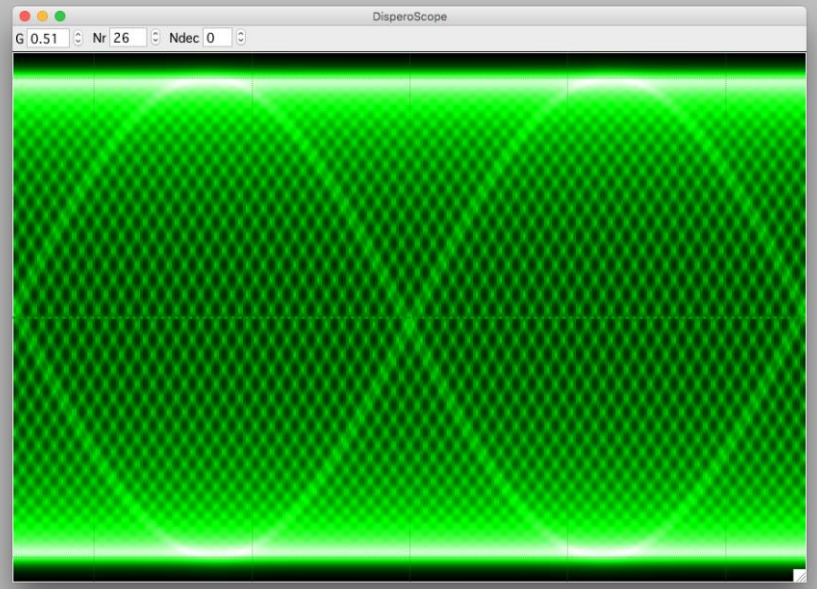




Commensurate *vs* Incommensurate

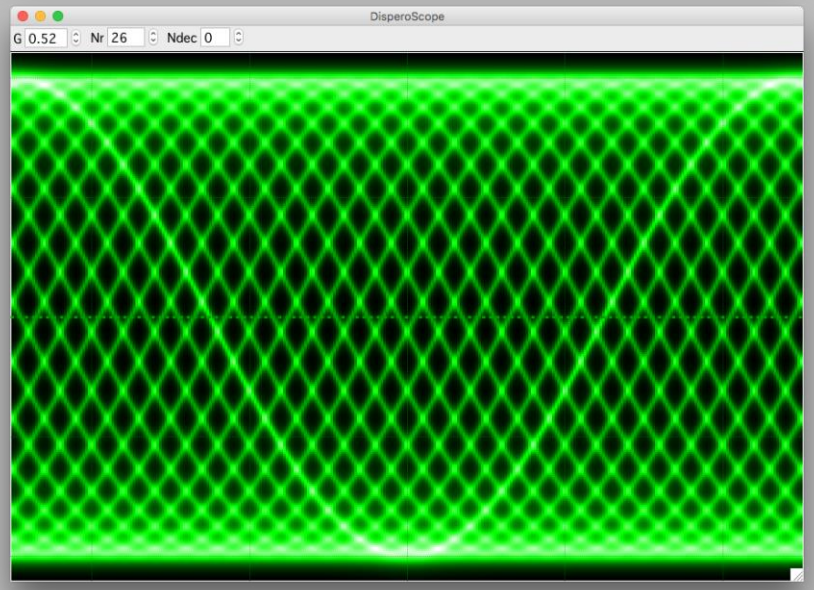


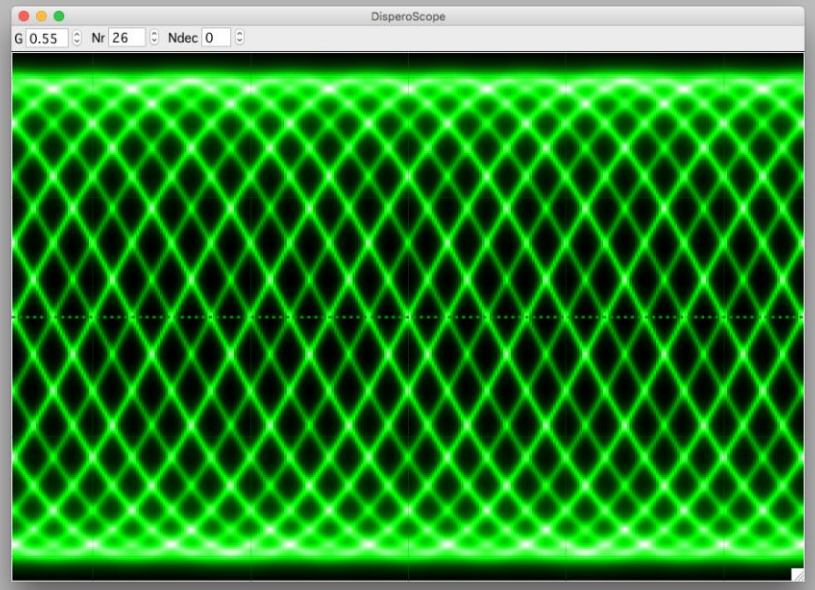




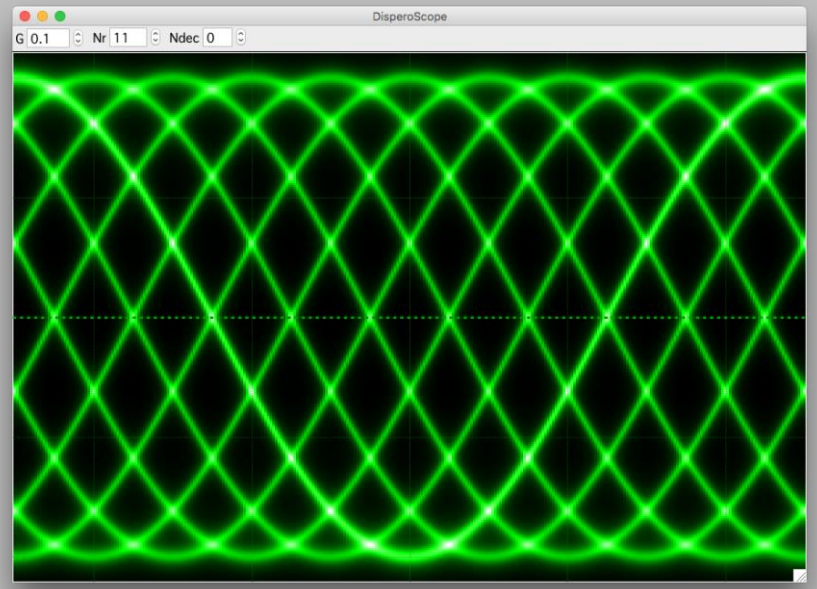
$$A(k,\omega) = \\ = \sum_{i=-(Nr-1)}^{Nr-1} \frac{1}{(\omega - \varepsilon_i(k))^2 + \delta^2}$$

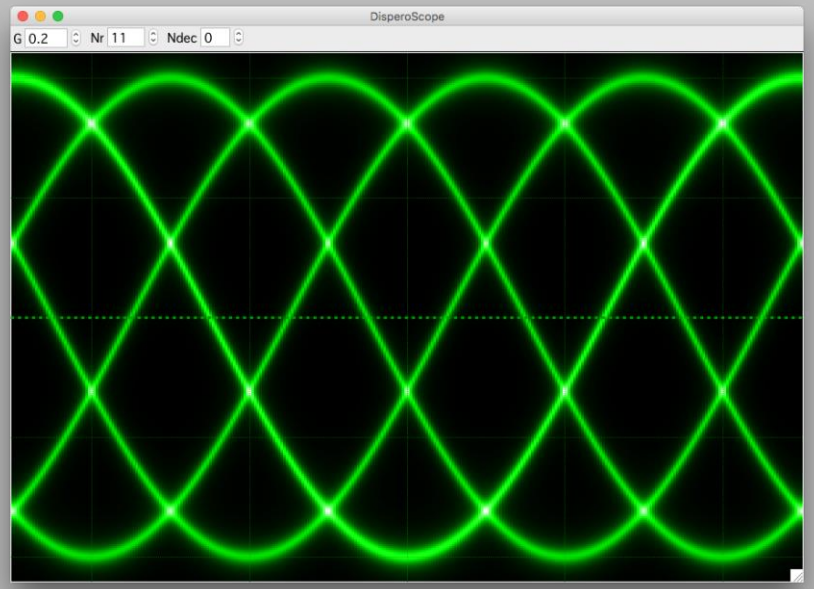
$$\varepsilon_i(k) = -\cos[2\pi(x + Gi)]$$

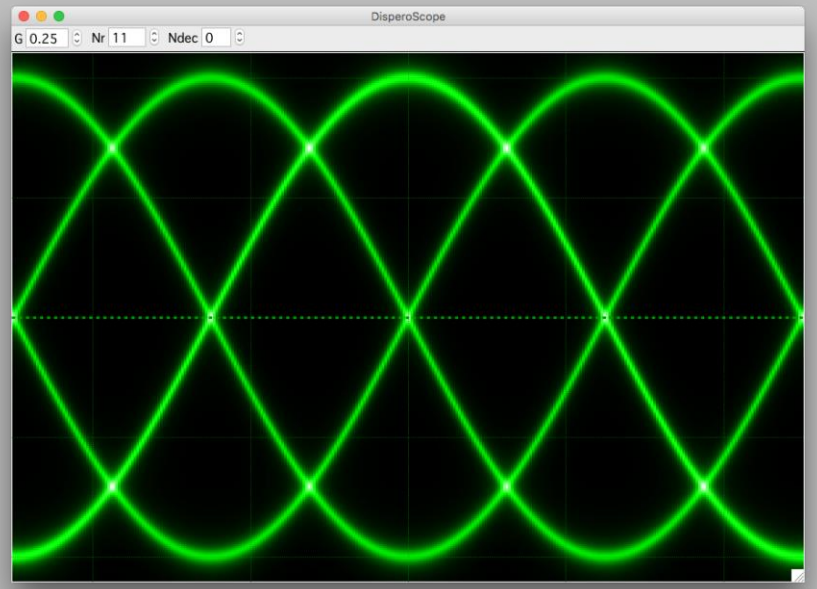


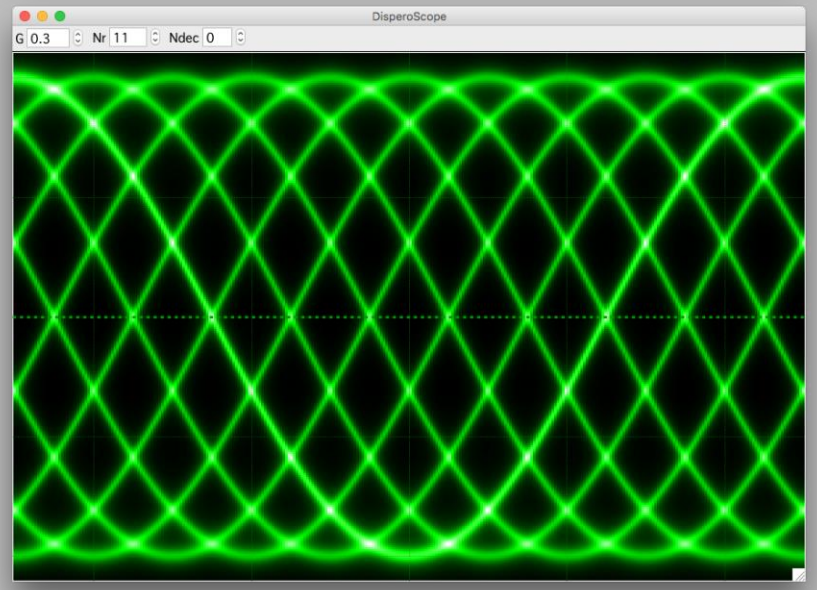


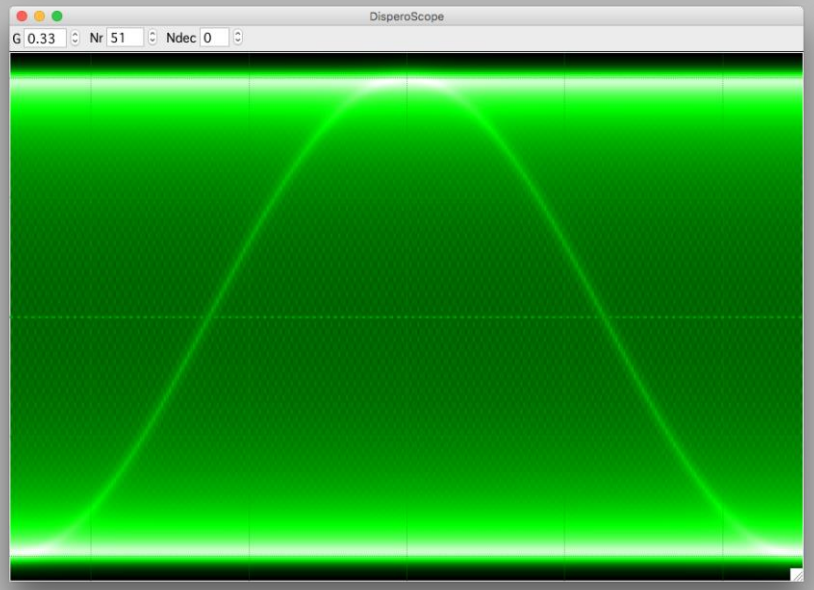
Commensurate *vs* Incommensurate

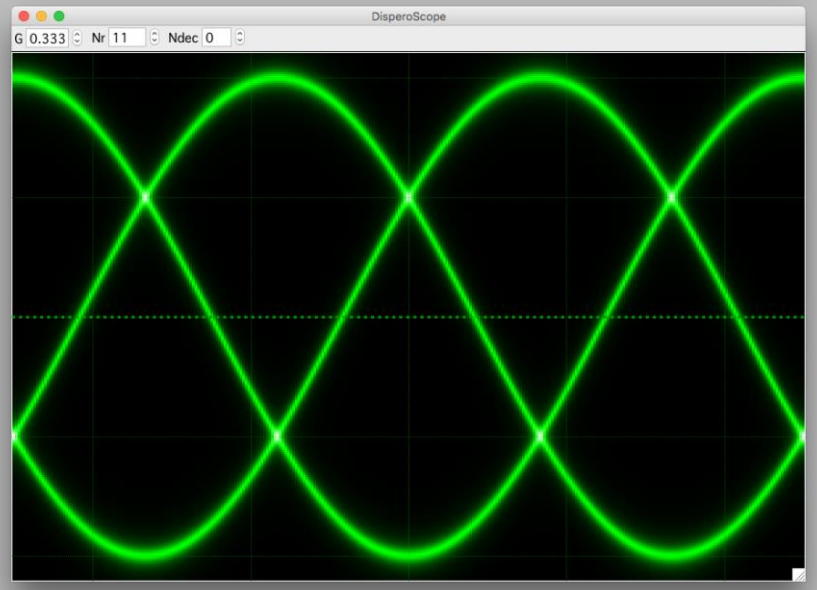




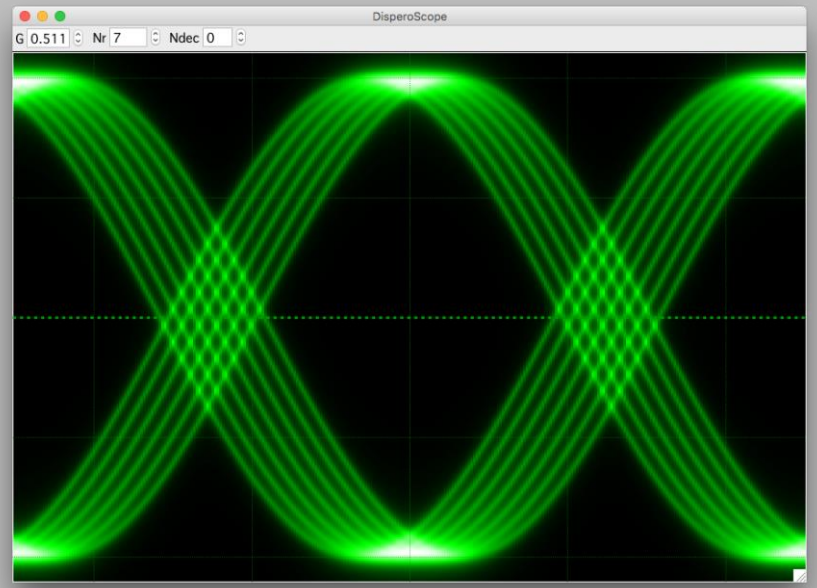


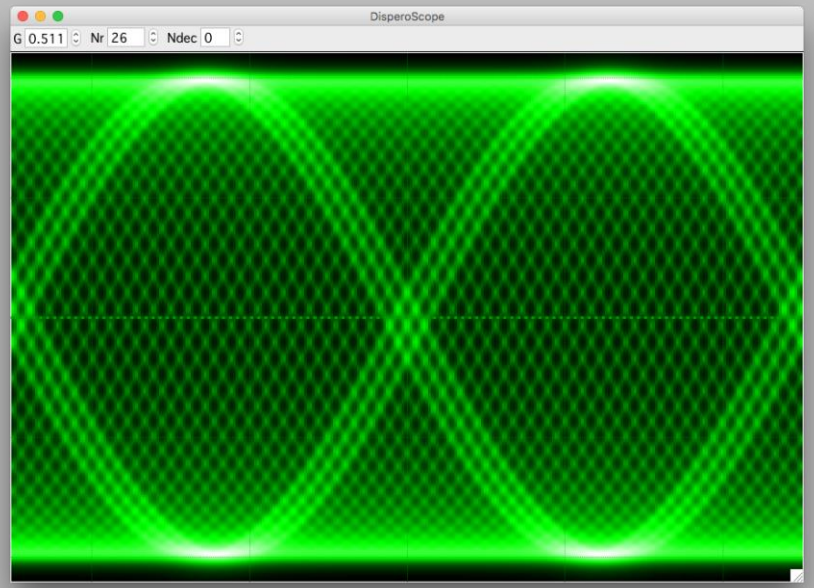


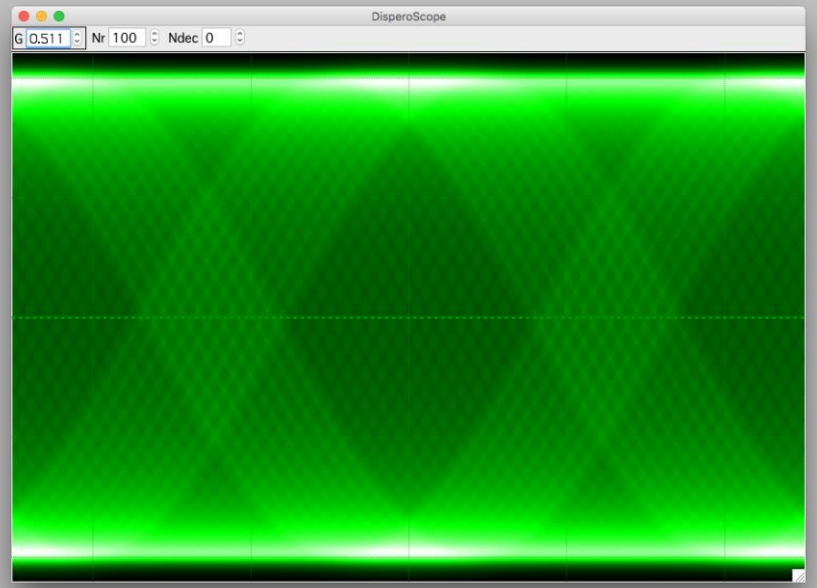




Commensurate *vs* Incommensurate

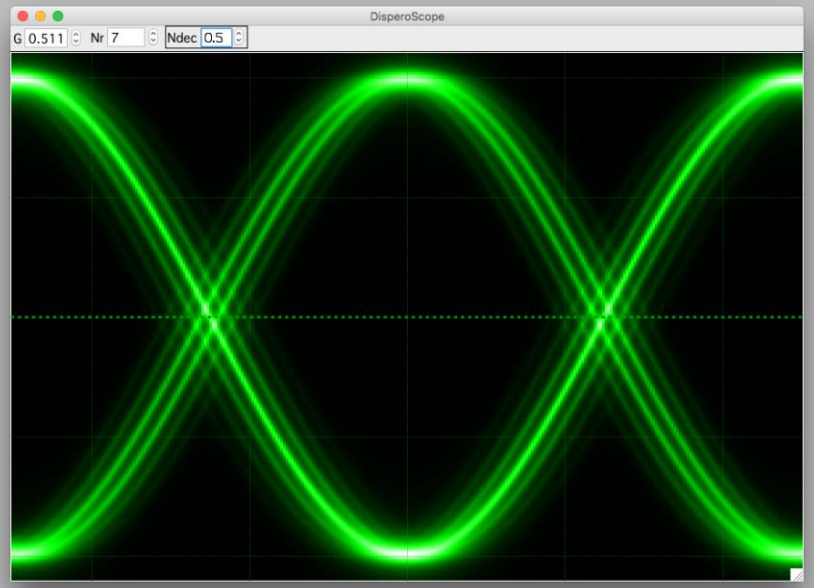


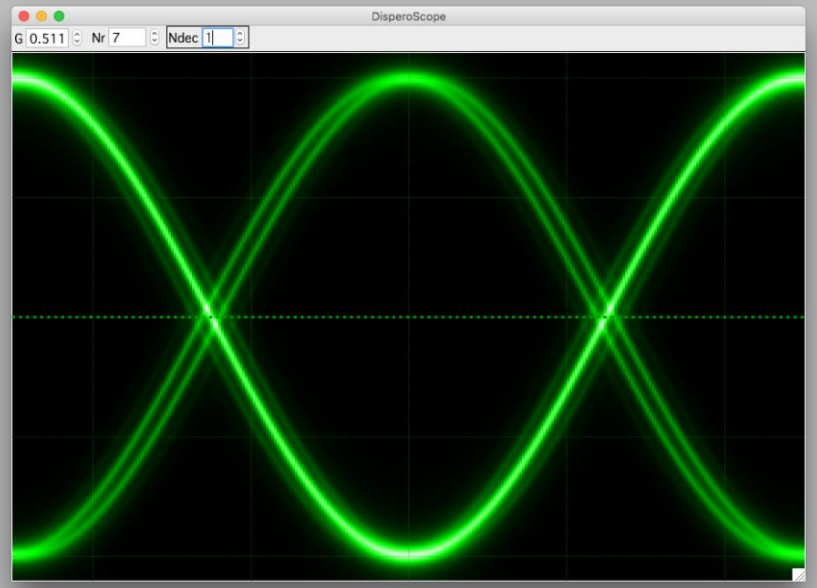


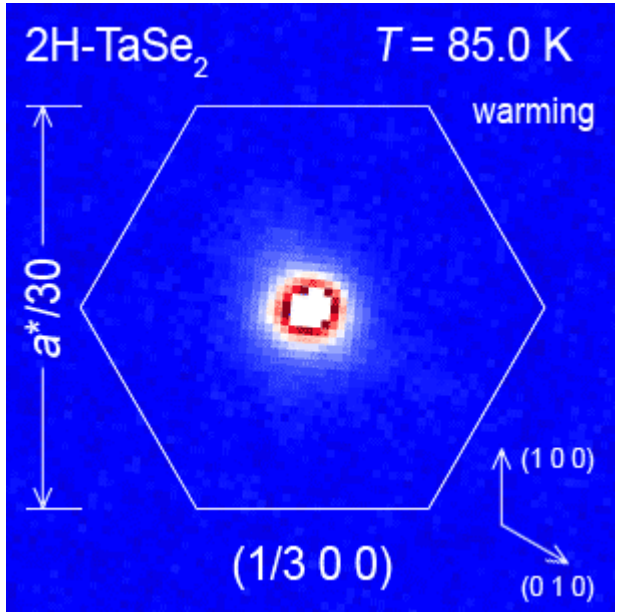


$$A(k,\omega) = \\ = \sum_{i=-(Nr-1)}^{Nr-1} \frac{\exp(-Di)}{(\omega - \varepsilon_i(k))^2 + \delta^2}$$

$$\varepsilon_i(k) = -\cos[2\pi(x + Gi)]$$

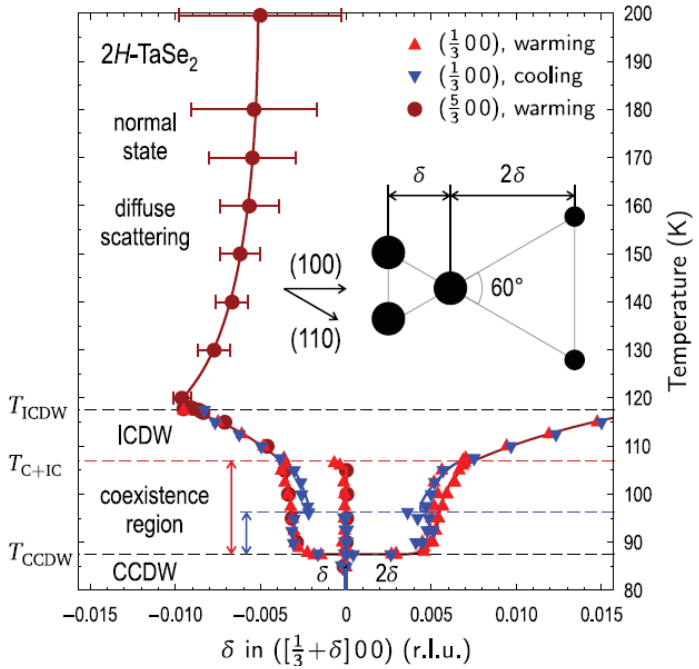


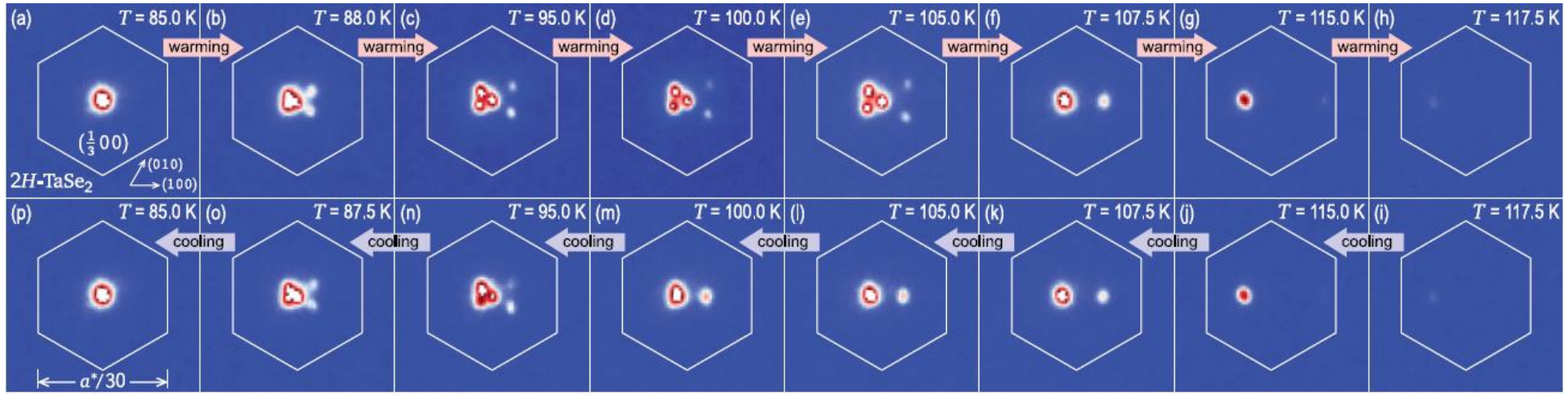




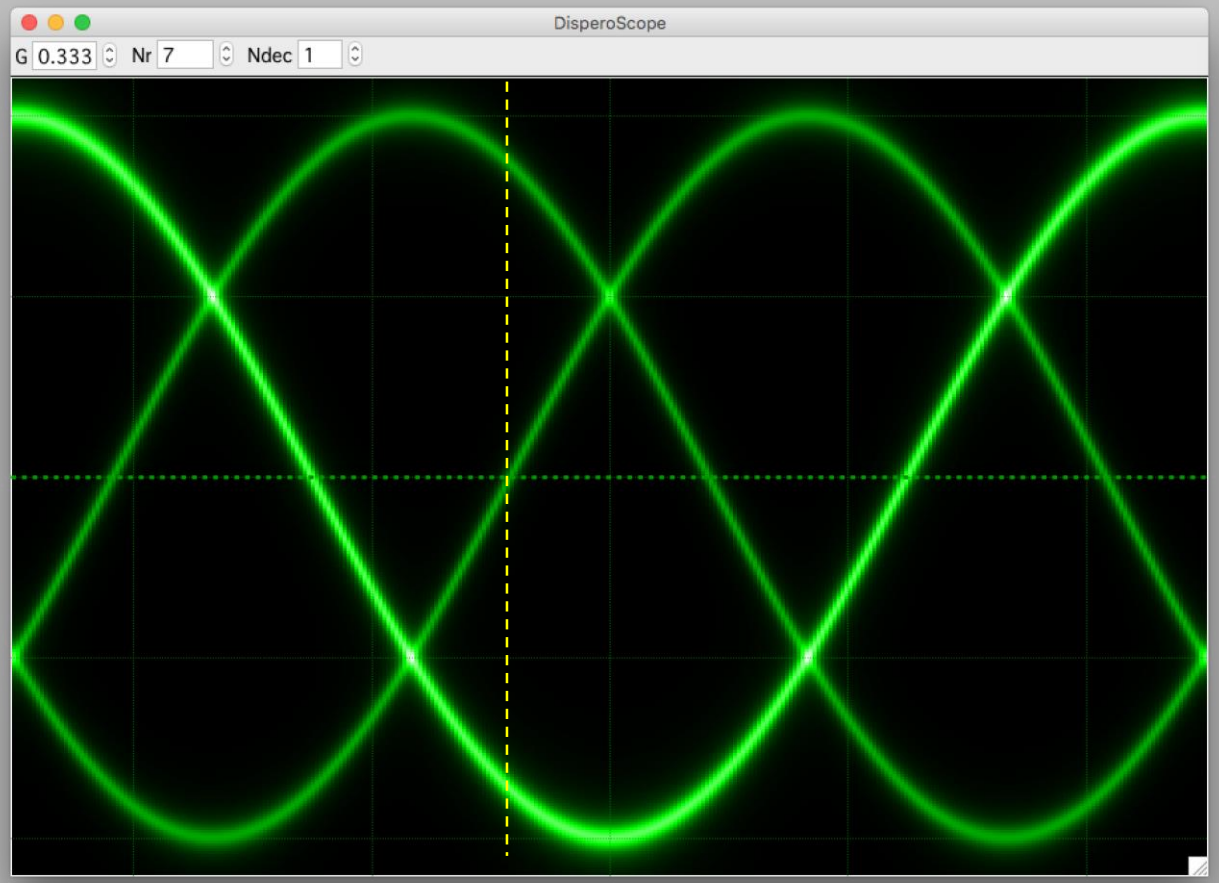
Competing CDW and temperature-dependent nesting in 2H-TaSe2

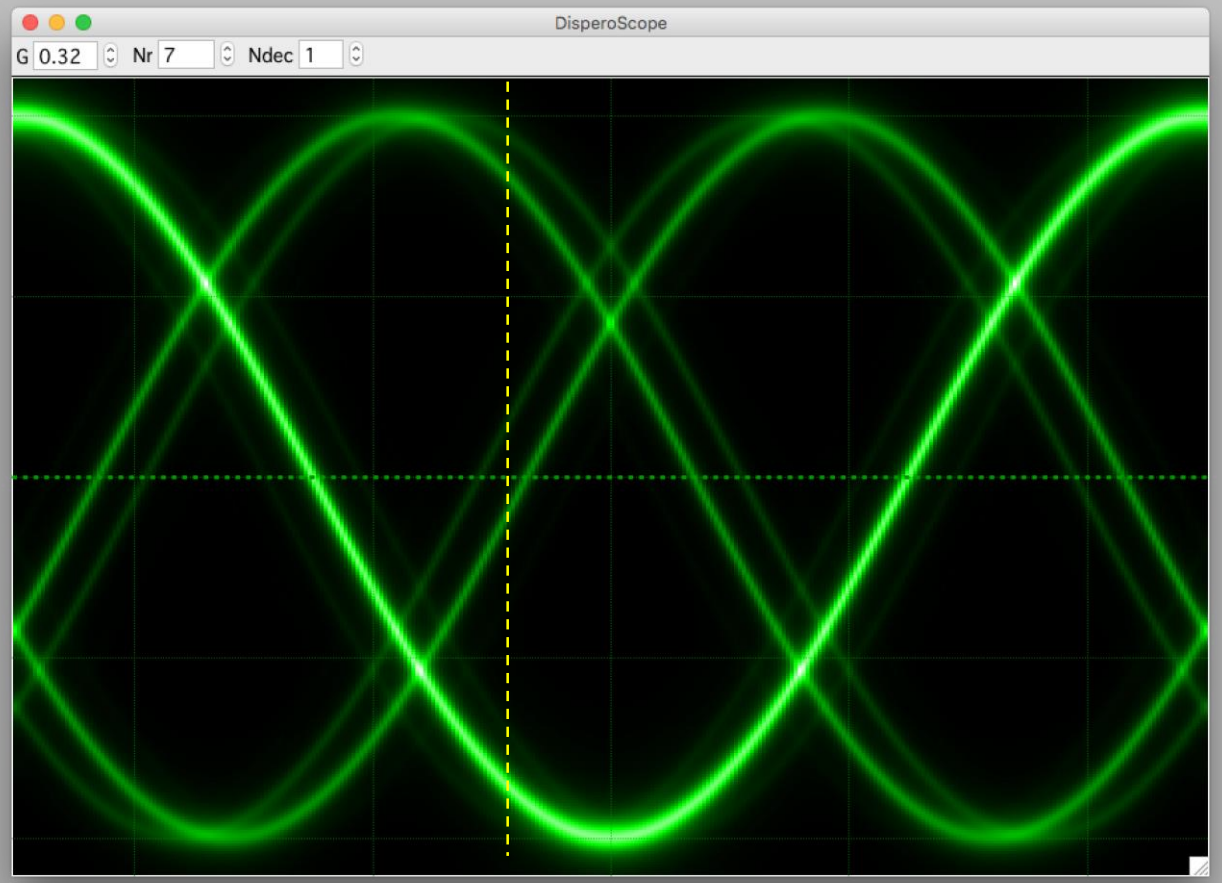
Leininger… Inosov, PRB 2011

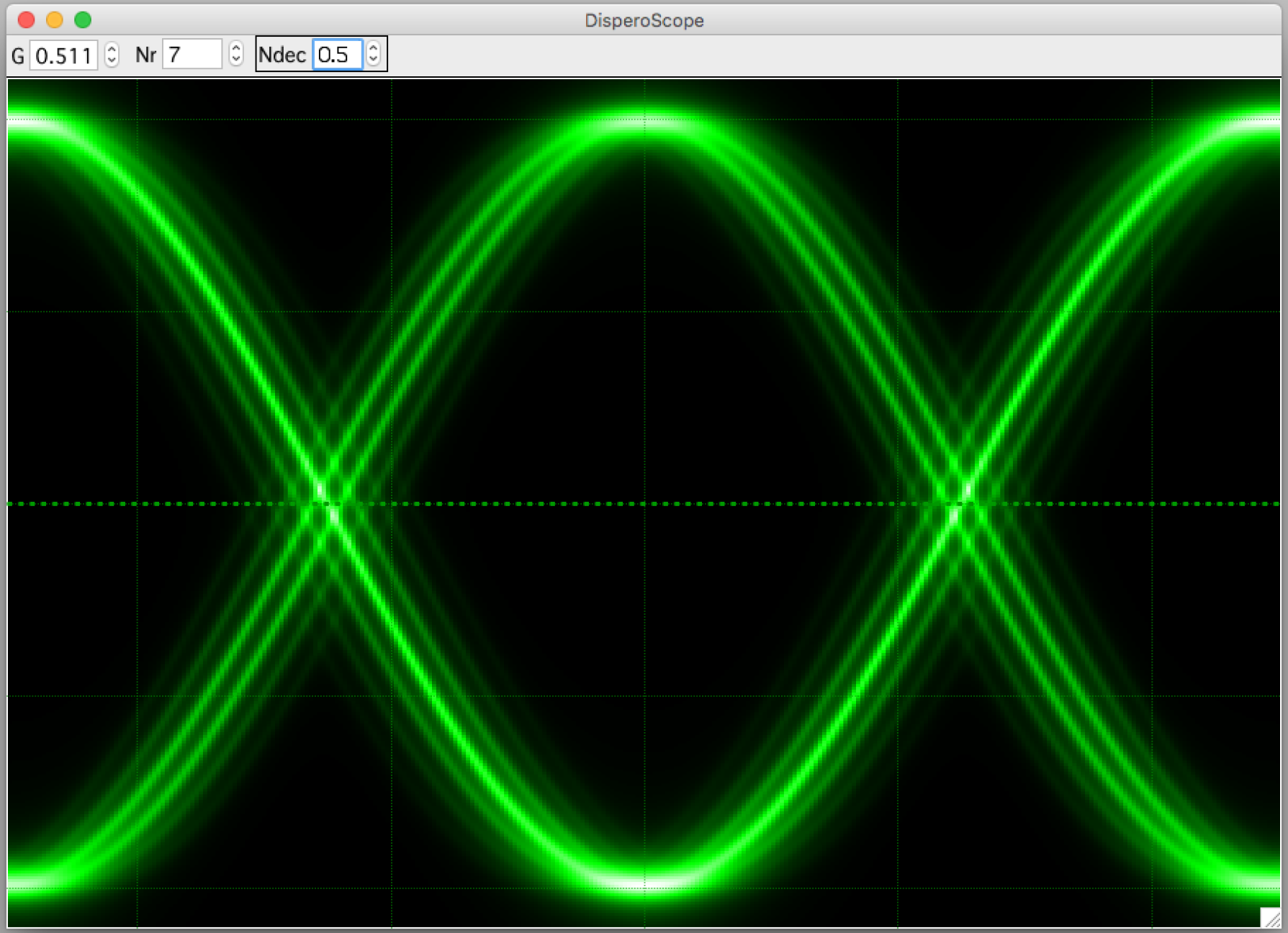




Commensurate *vs* Incommensurate

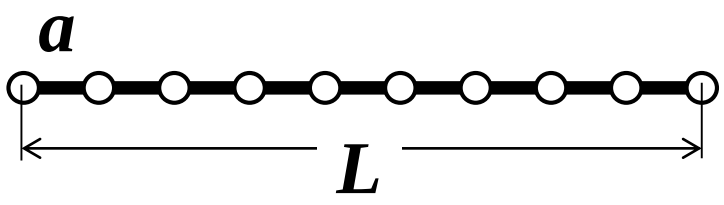


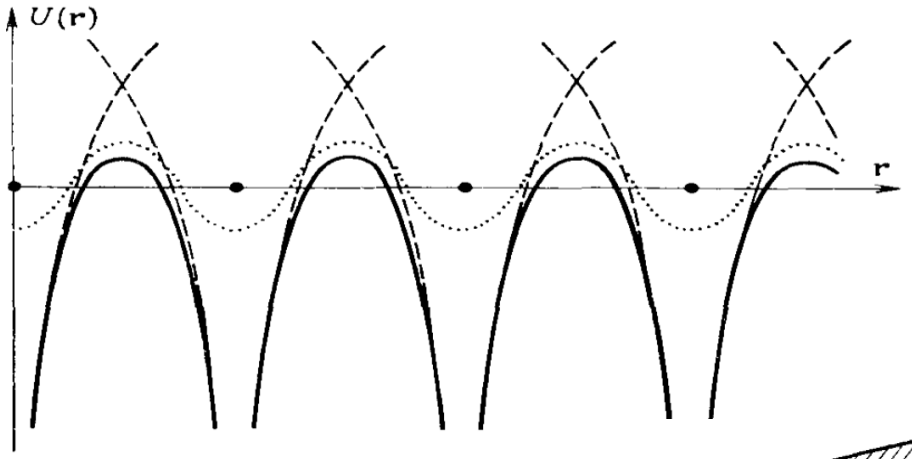


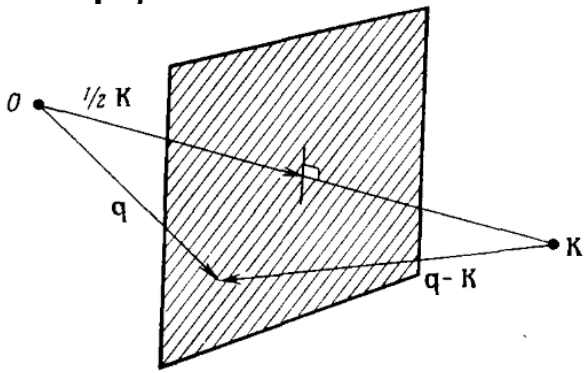

DisperoScope
G 0.511
Nr 7
Ndec 0.5

Band gaps

У попередніх лекціях…



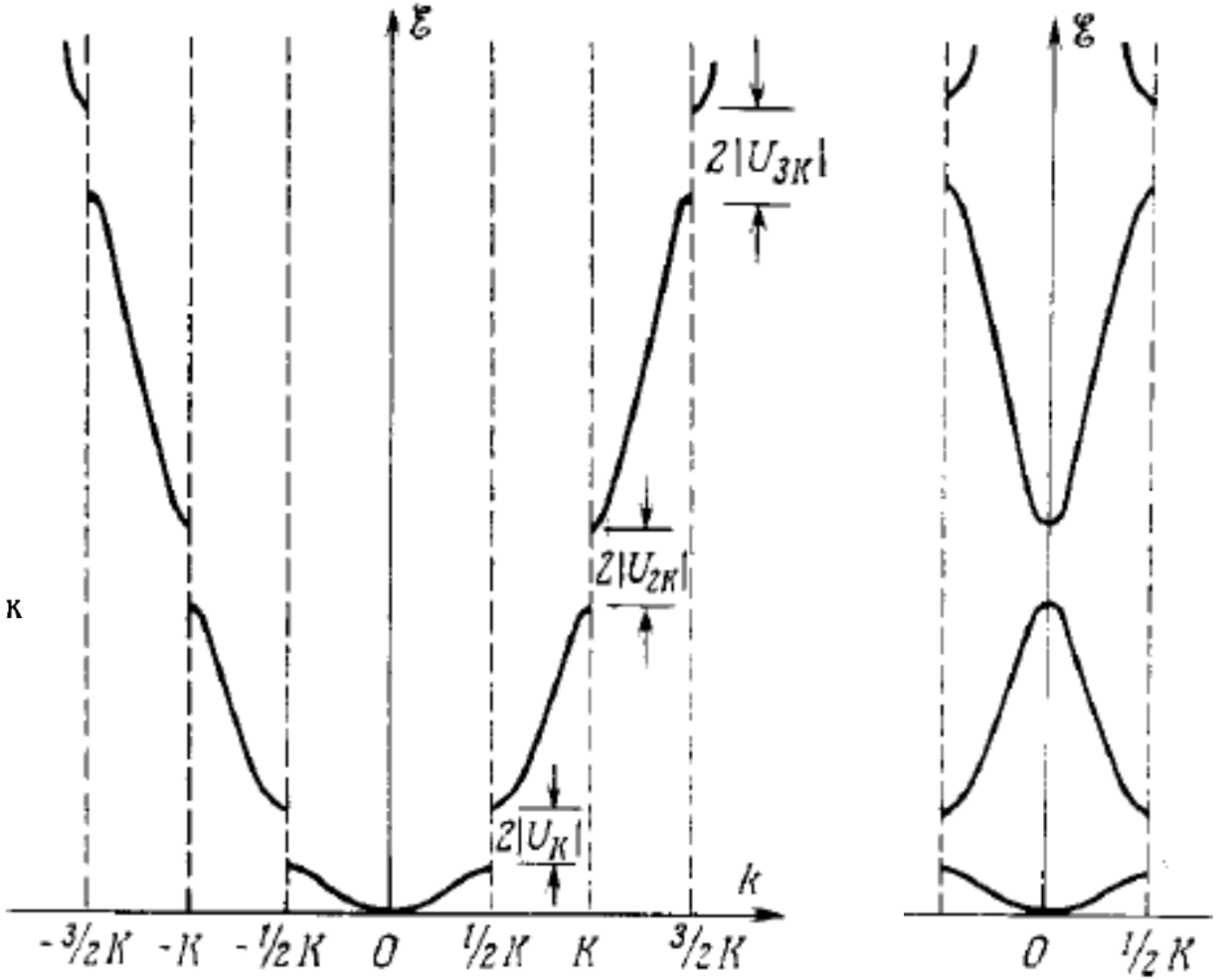




$$\begin{vmatrix} \mathscr{E} - \mathscr{E}^0_{\mathbf{q}} & -U_{\mathbf{K}} \\ -U^*_{\mathbf{K}} & \mathscr{E} - \mathscr{E}^0_{\mathbf{q}-\mathbf{K}} \end{vmatrix} = 0$$

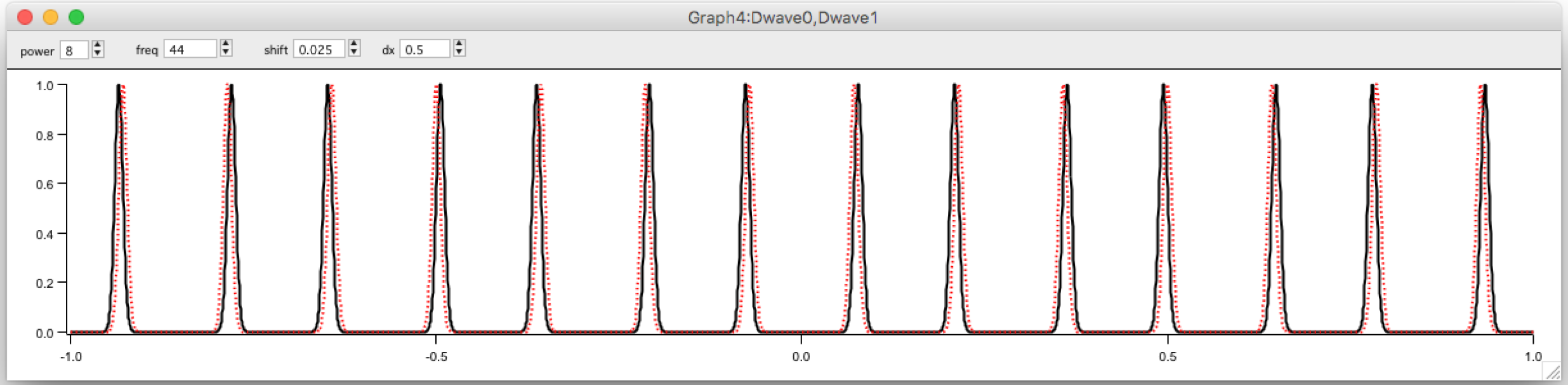
$$(\mathscr{E} - \mathscr{E}^0_{\mathbf{q}})(\mathscr{E} - \mathscr{E}^0_{\mathbf{q}-\mathbf{K}}) = |U_{\mathbf{K}}|^2$$

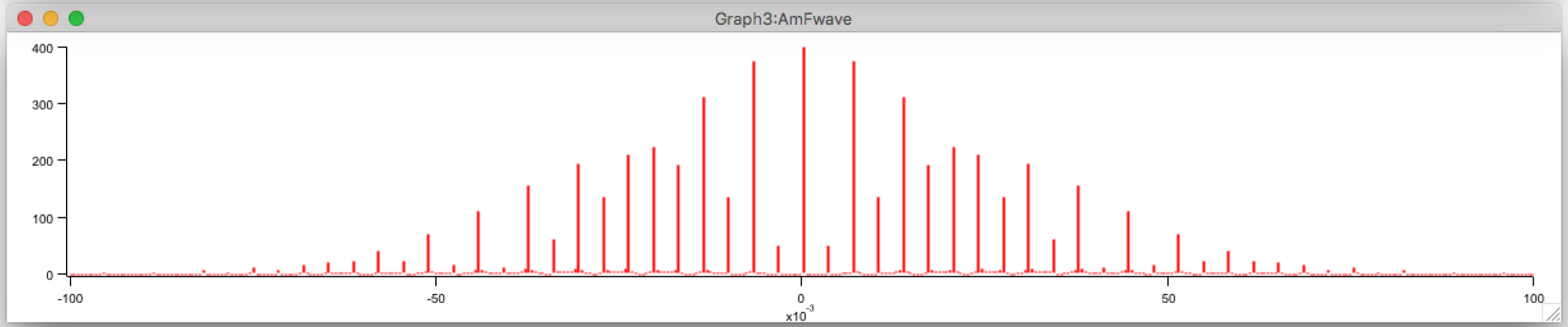
$$\mathscr{E} = \frac{1}{2}(\mathscr{E}^0_{\mathbf{q}} + \mathscr{E}^0_{\mathbf{q}-\mathbf{K}}) \pm \left[\left(\frac{\mathscr{E}^0_{\mathbf{q}} - \mathscr{E}^0_{\mathbf{q}-\mathbf{K}}}{2}\right)^2 + |U_{\mathbf{K}}|^2\right]^{1/2}$$



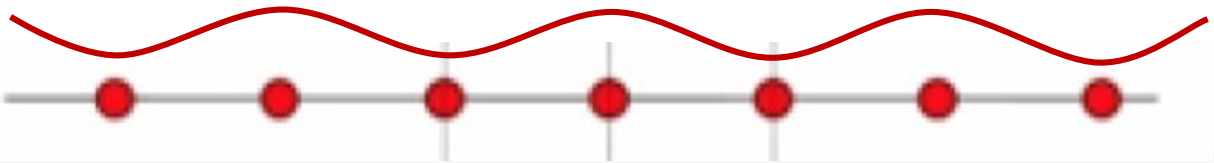
$K = 2\pi/a$

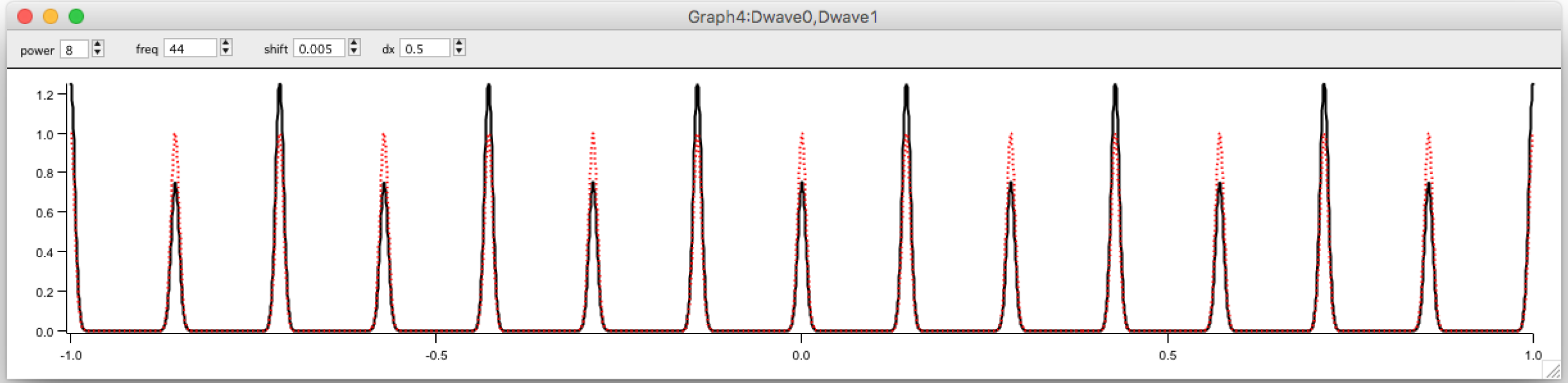
CDW band gaps

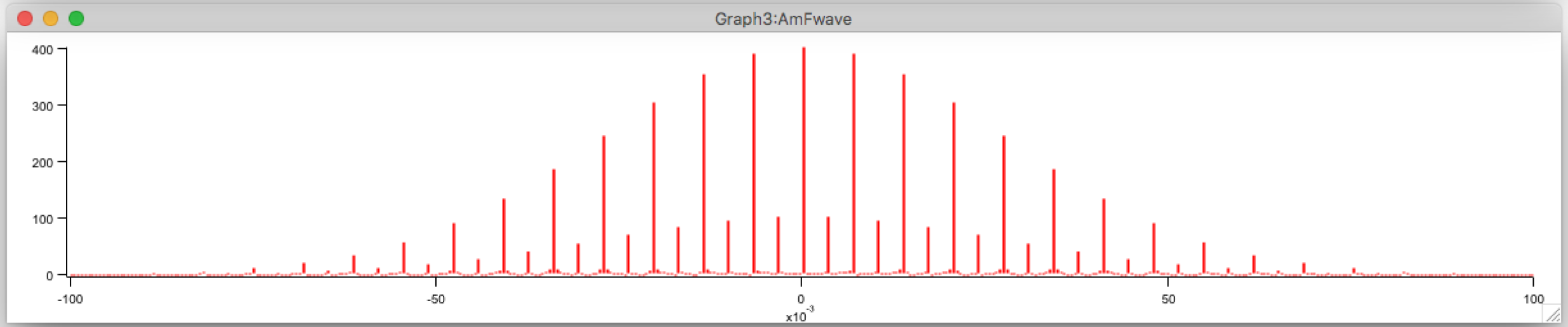




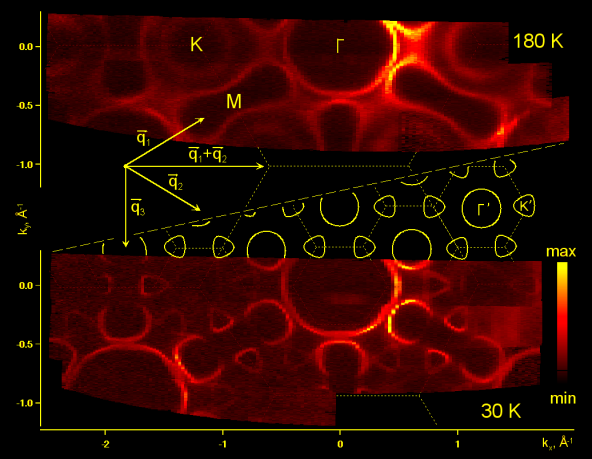
CDW band gaps

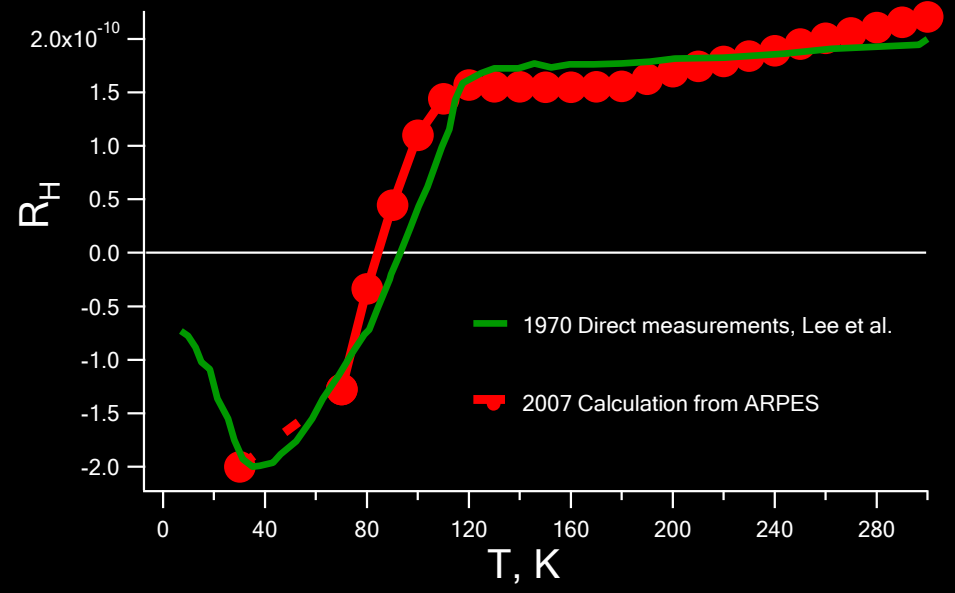






Hall coefficient of 2H-$TaSe_2$ from ARPES



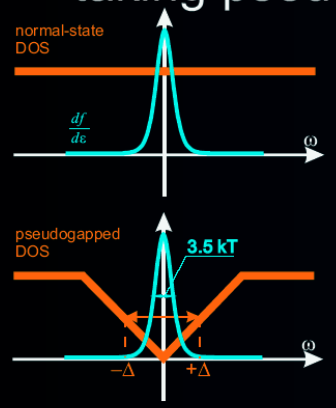


Hall coefficient from electronic structure

$$\tau(\mathbf{k}) = \text{const}$$

$$R_H = \frac{\sigma_{xy}}{H \cdot \sigma_{xx}^2} = \frac{\int \tau(\mathbf{k})^2 \cdot \frac{v_F^2(\mathbf{k})}{\rho(\mathbf{k})} \cdot dk}{\left(\int \tau(\mathbf{k}) \cdot v_F(\mathbf{k}) \cdot dk\right)^2} = \frac{\int \frac{v_F^2(\mathbf{k})}{\rho(\mathbf{k})} \cdot dk}{\left(\int v_F(\mathbf{k}) \cdot dk\right)^2}$$

taking pseudogap into account



$$D(\mathbf{k}) = -\int_{-\infty}^{\infty} \frac{df}{d\varepsilon} \cdot A(\varepsilon, \mathbf{k}) \cdot d\varepsilon \le 1$$

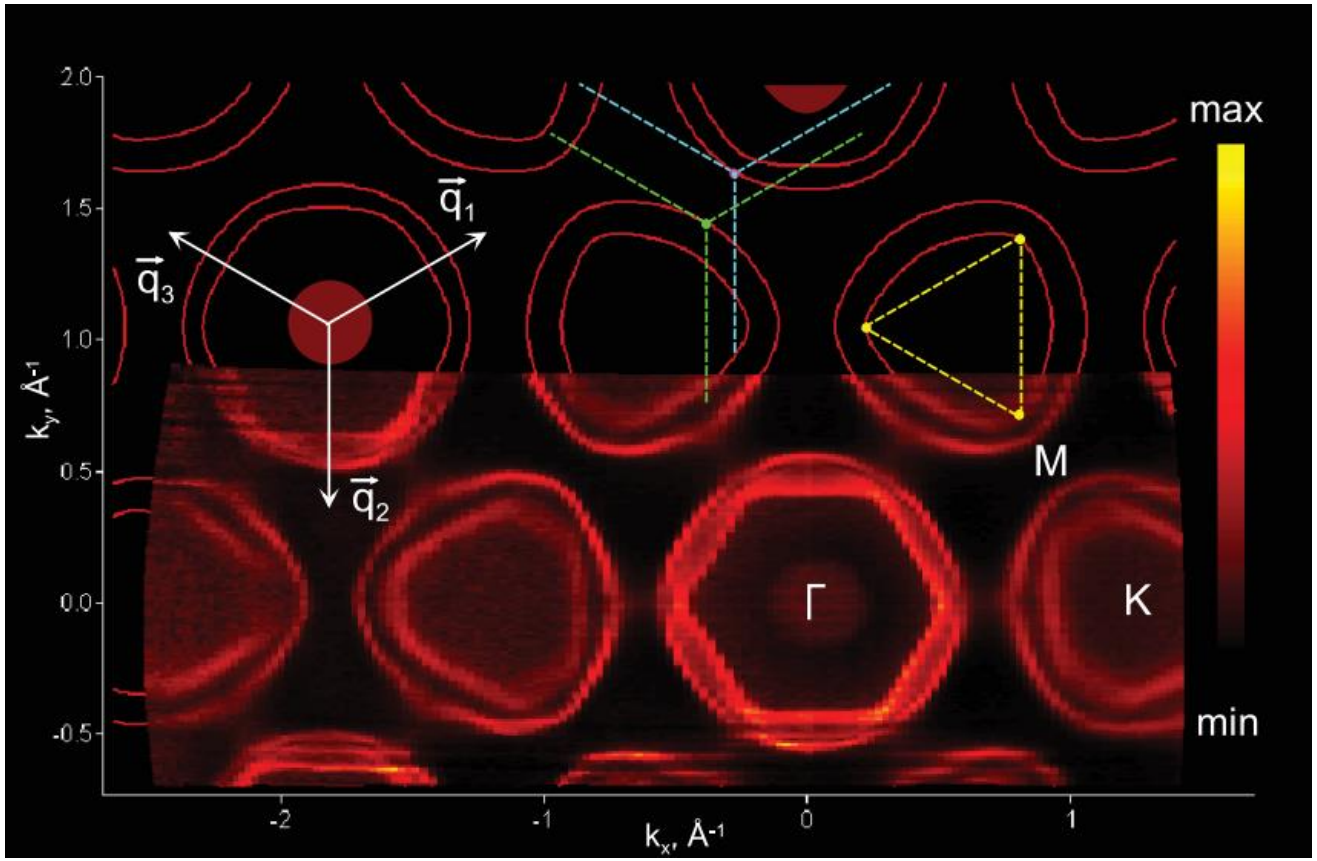
$$\sigma_{xy} \propto \int D(\mathbf{k}) \cdot \frac{\tau^2(\mathbf{k}) \cdot v_F^2(\mathbf{k})}{\rho(\mathbf{k})} \cdot dk$$

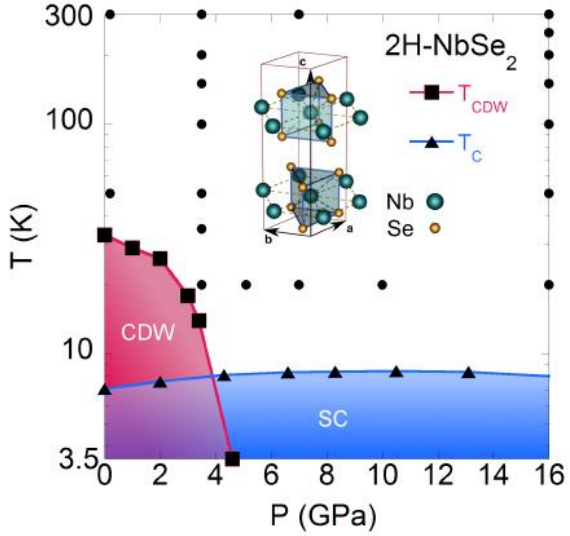
Evtushinsky *PRL* 2008

PRL 102, 166402 (2009) PHYSICAL REVIEW LETTERS week ending 24 APRIL 2009

Two Energy Gaps and Fermi-Surface "Arcs" in $NbSe_2$

S. V. Borisenko,[1] A. A. Kordyuk,[1] V. B. Zabolotnyy,[1] D. S. Inosov,[1] D. Evtushinsky,[1] B. Büchner,[1] A. N. Yaresko,[2] A. Varykhalov,[3] R. Follath,[3] W. Eberhardt,[3] L. Patthey,[4] and H. Berger[5]





Leroux PRB 2015

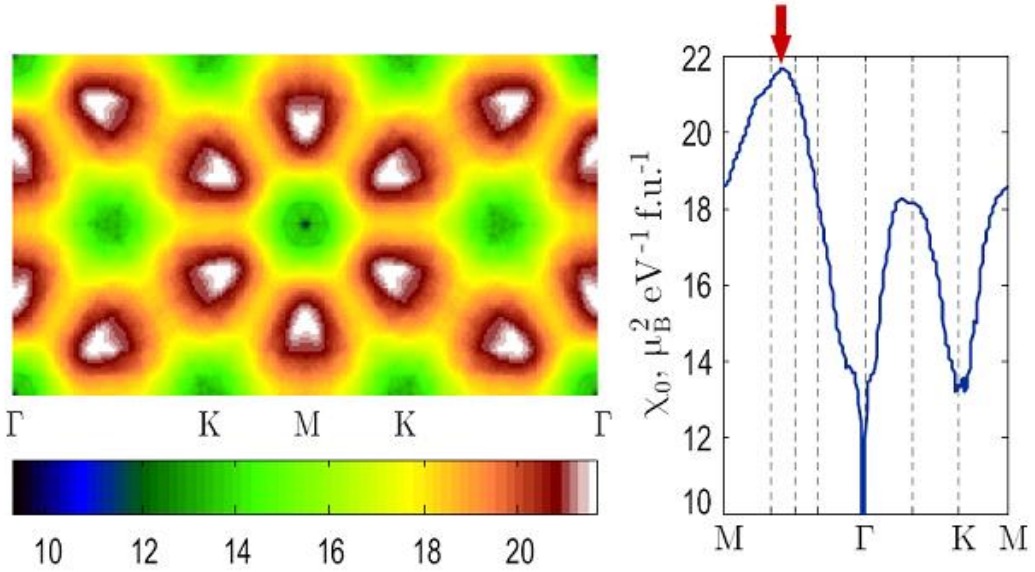
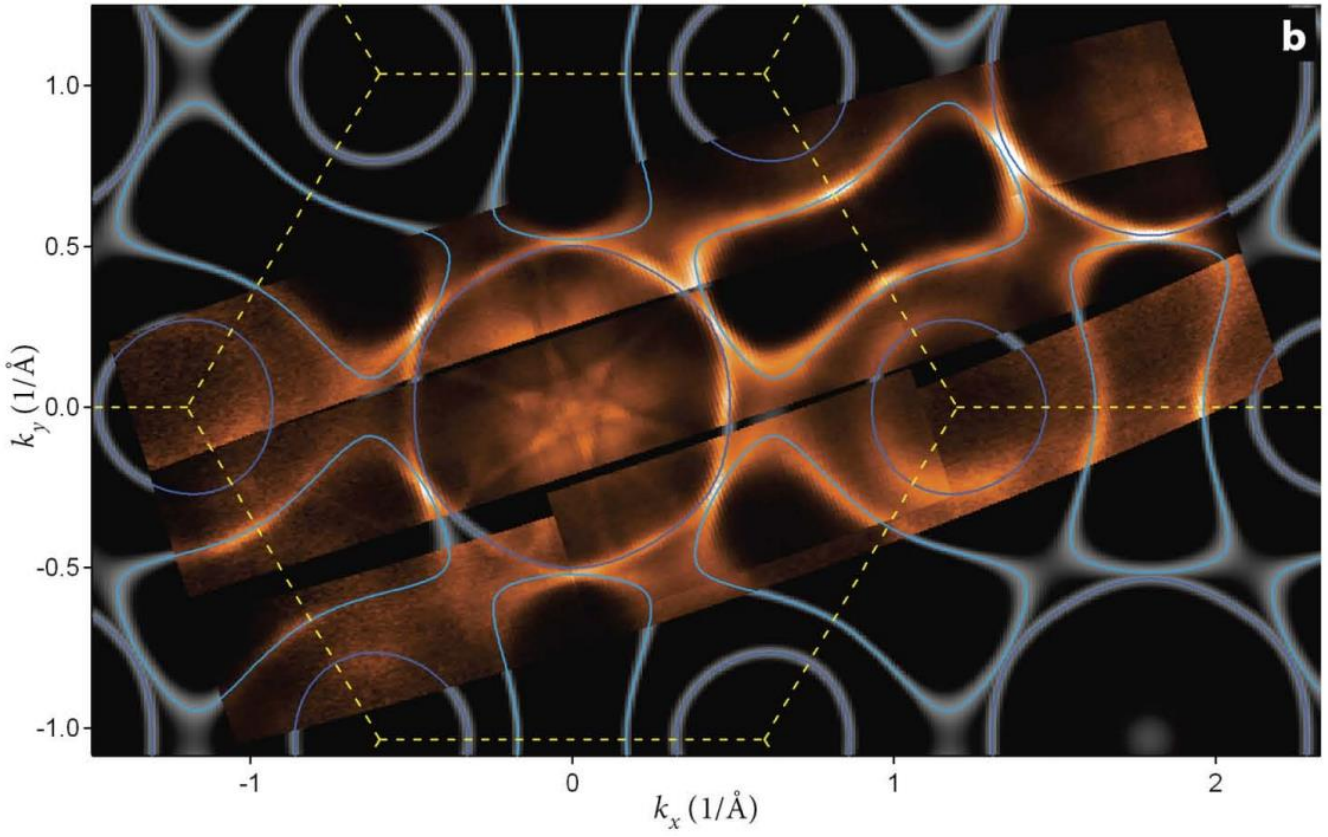
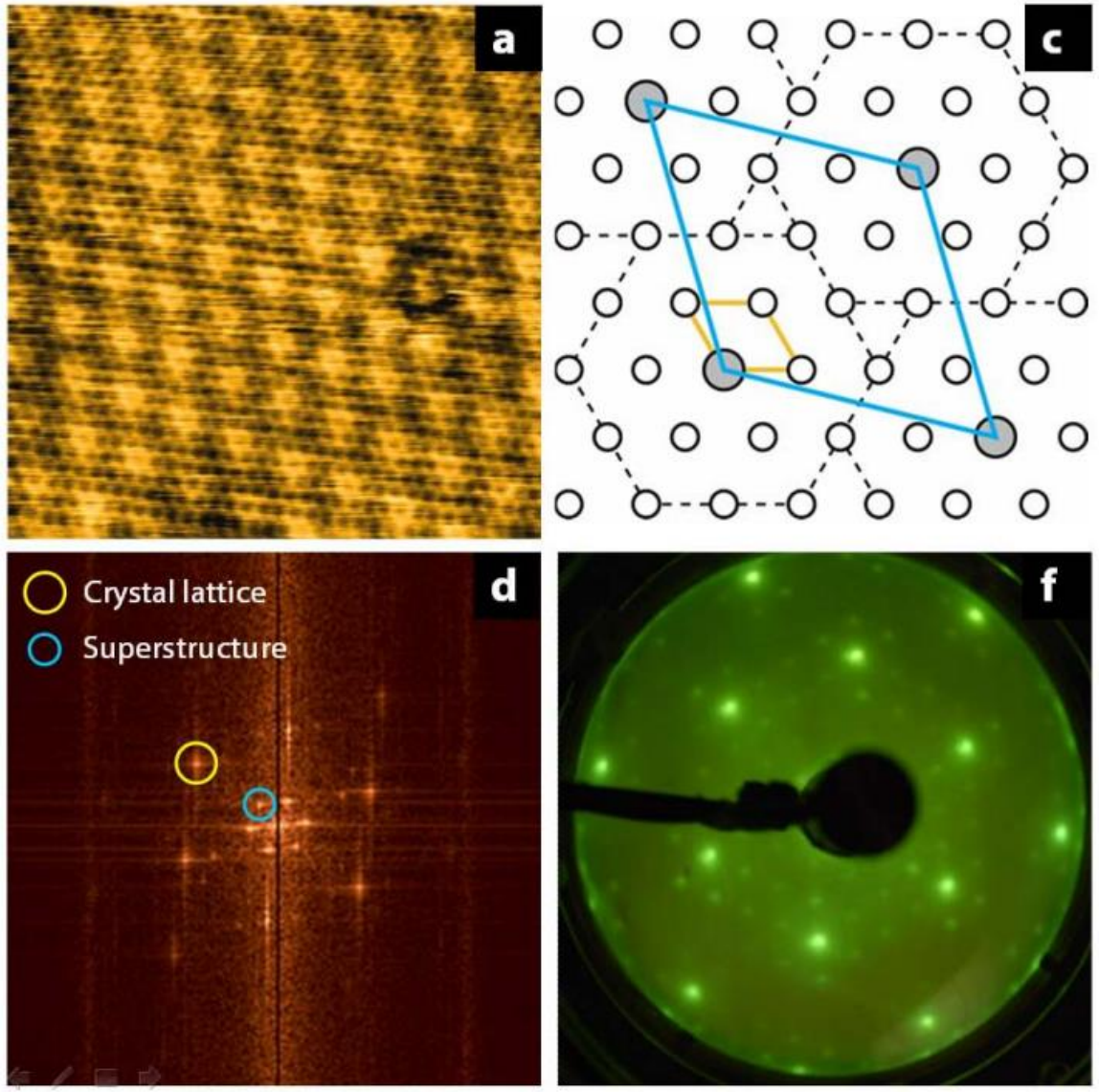


Figure S2. Real part of the Lindhard function at ω → 0 as a function of momentum and corresponding profile along high-symmetry directions, with the dominant nesting vector marked by the red arrow. The same vectors can be seen in left panel as white spots.





Cu-intercalated 2H-TaSe2

-> 2Hb-TaSe2

Quasicrystals

Квазікристал [ред. | ред. код]

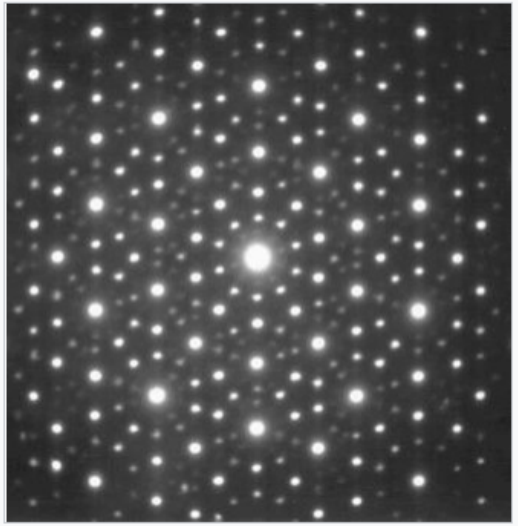
Матеріал з Вікіпедії — вільної енциклопедії.

Квазікристал — це тверде тіло, атоми якого впорядковані так, що не утворюють кристалічної ґратки (тобто ця структура не є періодичною, позбавлена трансляційної симетрії), але в той же час можуть когерентно розсіювати випромінювання.

Найважливішою рисою квазікристалів є те, що вони дають чіткі бреґґівські піки при дифракції рентгенівських променів і електронів, причому осі симетрії цих піків мають заборонені для кристалів порядки, наприклад 5-ий. В загальному ж випадку неперіодична структура (наприклад, аморфне тіло, рідина тощо), не обов'язково дає чіткі бреґґвські піки.

Є два типи квазікисталів: 1) структура періодична по одній осі, а у площині перпендикулярній до цій осі — квазікристалічна; 2) структура квазікристалічна в усіх трьох напрямках.

Здебільшого квазікристали утворюються при швидкому охолодженні розплавлених сплавів металів (Al-Li-Cu, Al-Mn-Si, Al-Ni-Co, Al-Pd-Mn, Al-Cu-Fe, Al-Cu-V, Cd-Yb, Ti-Zr-Na, Zn-Mg-Ho, Zn-Mg-Sc, In-Ag-Yb, Pd-U-Si тощо), і є нестабільними, однак виявлені також стабільні квазікристалічні речовини.



Дифракційна картина розсіяння електронів на ікосаедричній структурі квазікристалу Zn-Mg-Ho. Видно 10 точок по колу.

Історія [ред. | ред. код]

Математично можливість заповнення простору кількома простими комірками з утворенням неперіодичної структури відкрив у 1970-их Роджер Пенроуз.

Квазікристали були відкриті в 1984 році Даном Шехтманом.

Деякі приклади нерекурсивної математики

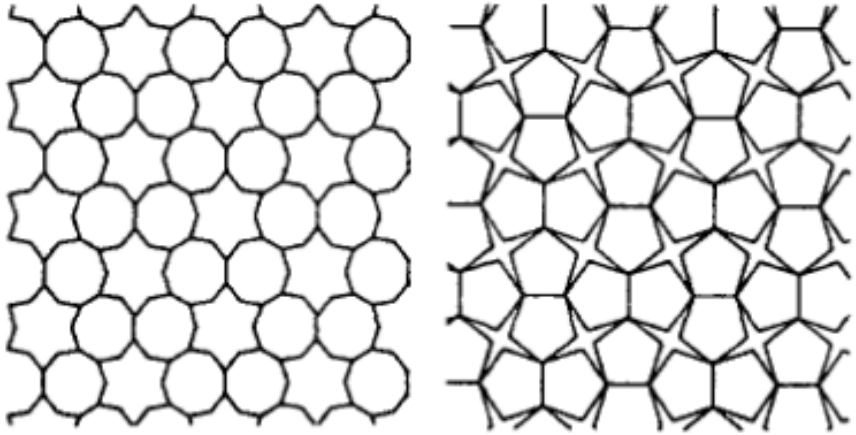


Рис. 4.7. Два примера периодического замощения плоскости фигурами двух форм

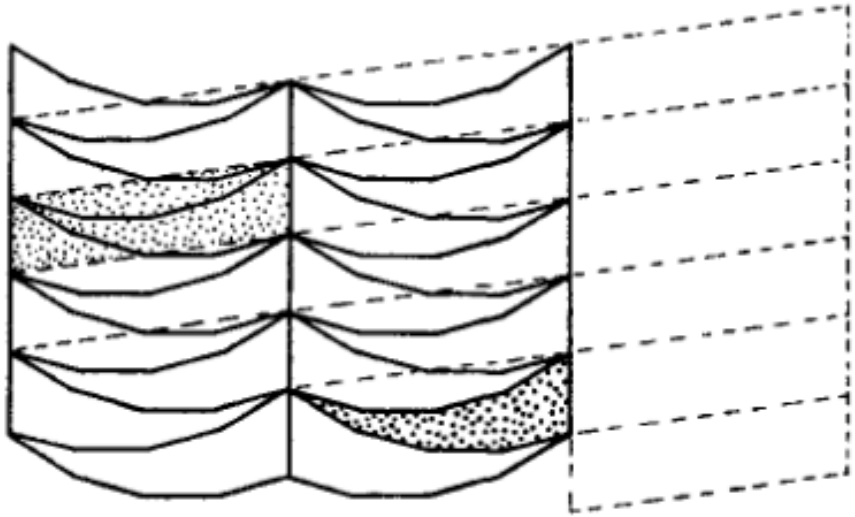


Рис. 4.8. Периодическое замощение и его параллелограмм периодов

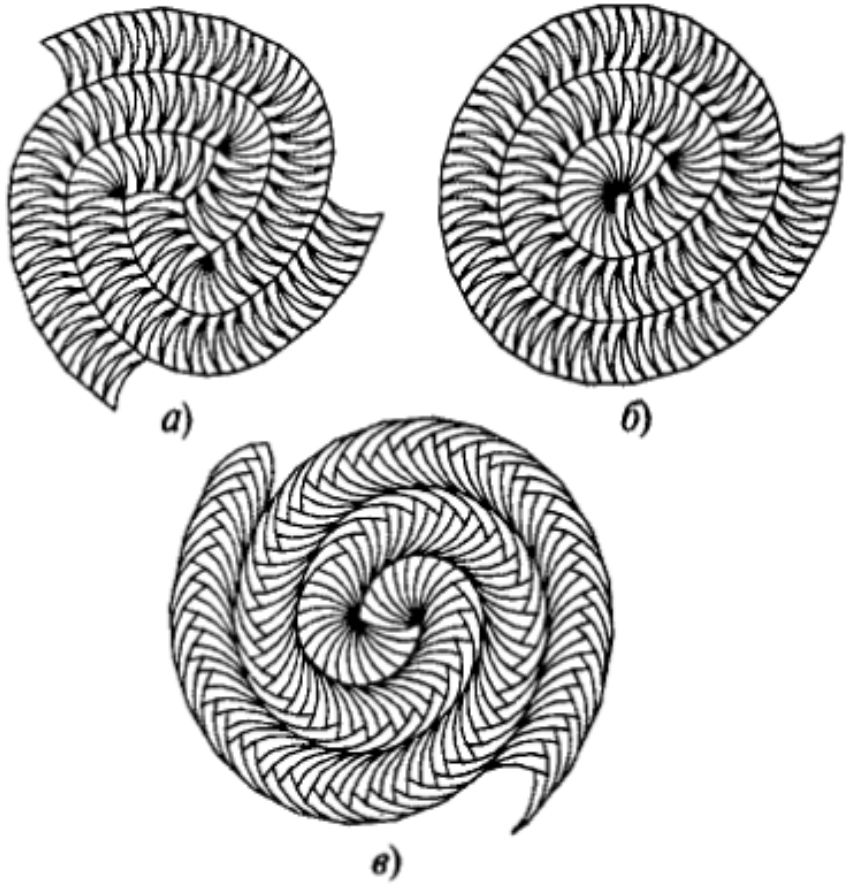
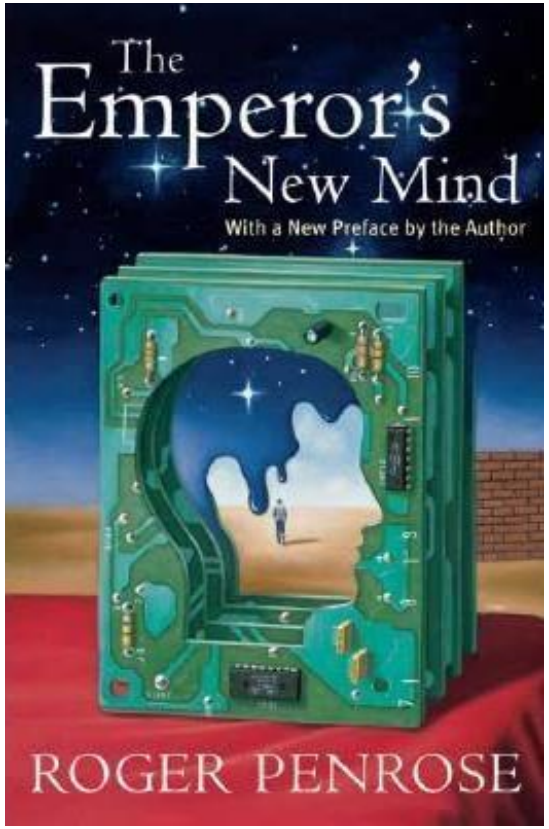


Рис. 4.9. Три непериодических «спиральных» замощения из таких же «универсальных» плиток, как и на рис. 4.8



Пенроуз Р. Новый ум короля.djvu

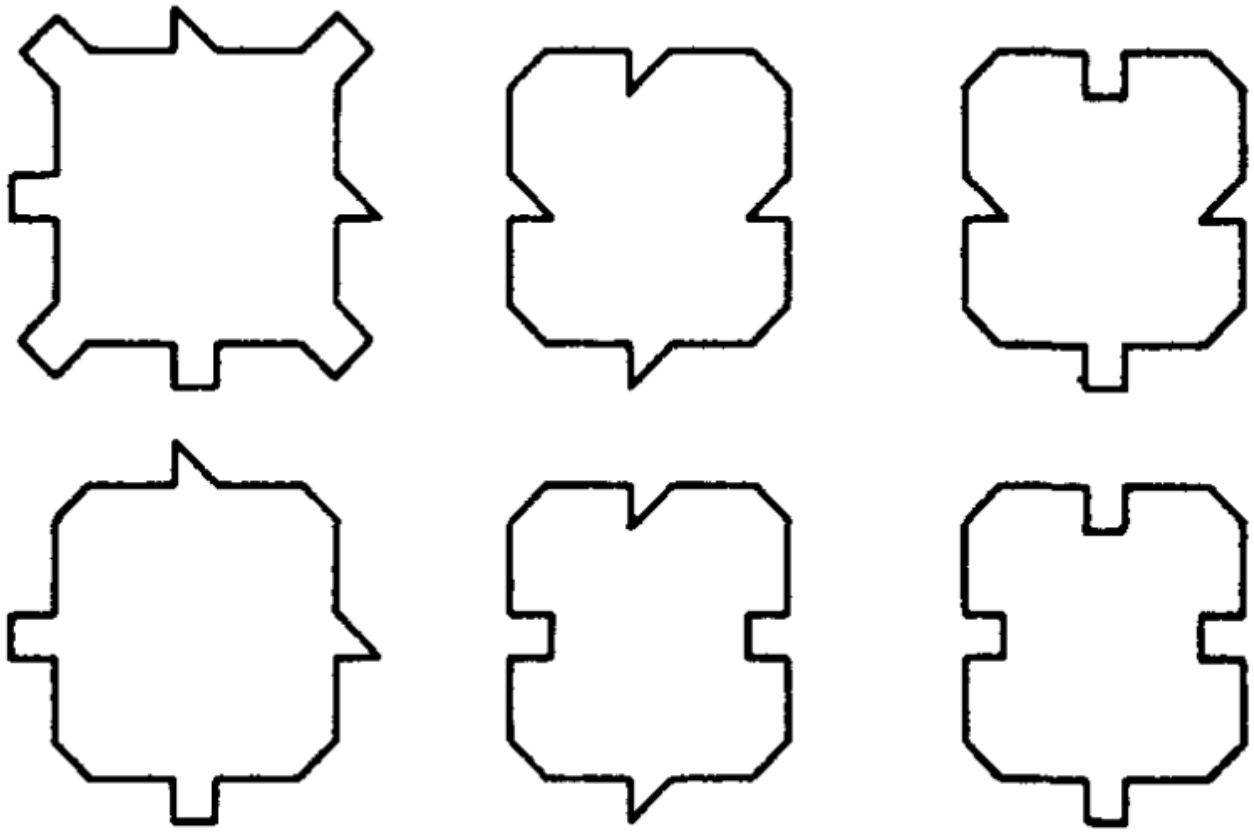
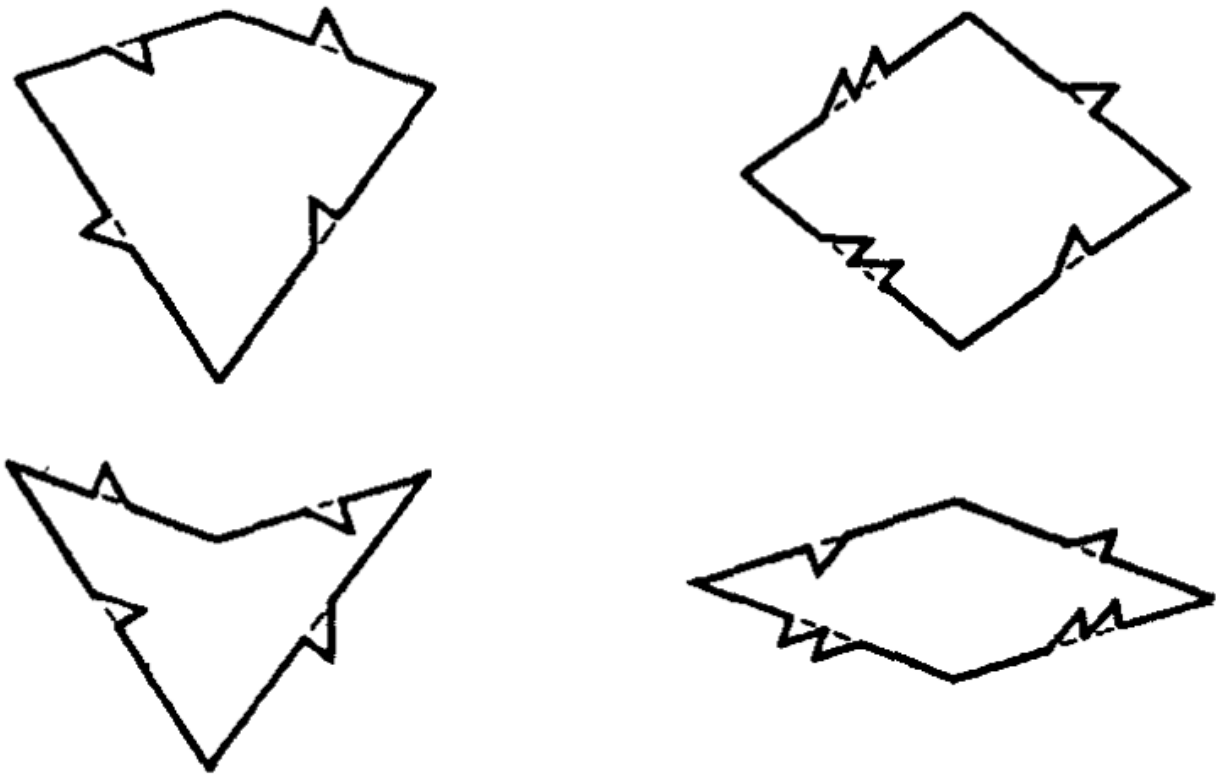


Рис. 4.10. Набор Рафазля Робинсона из шести плиток, который покрывает плоскость только непериодически



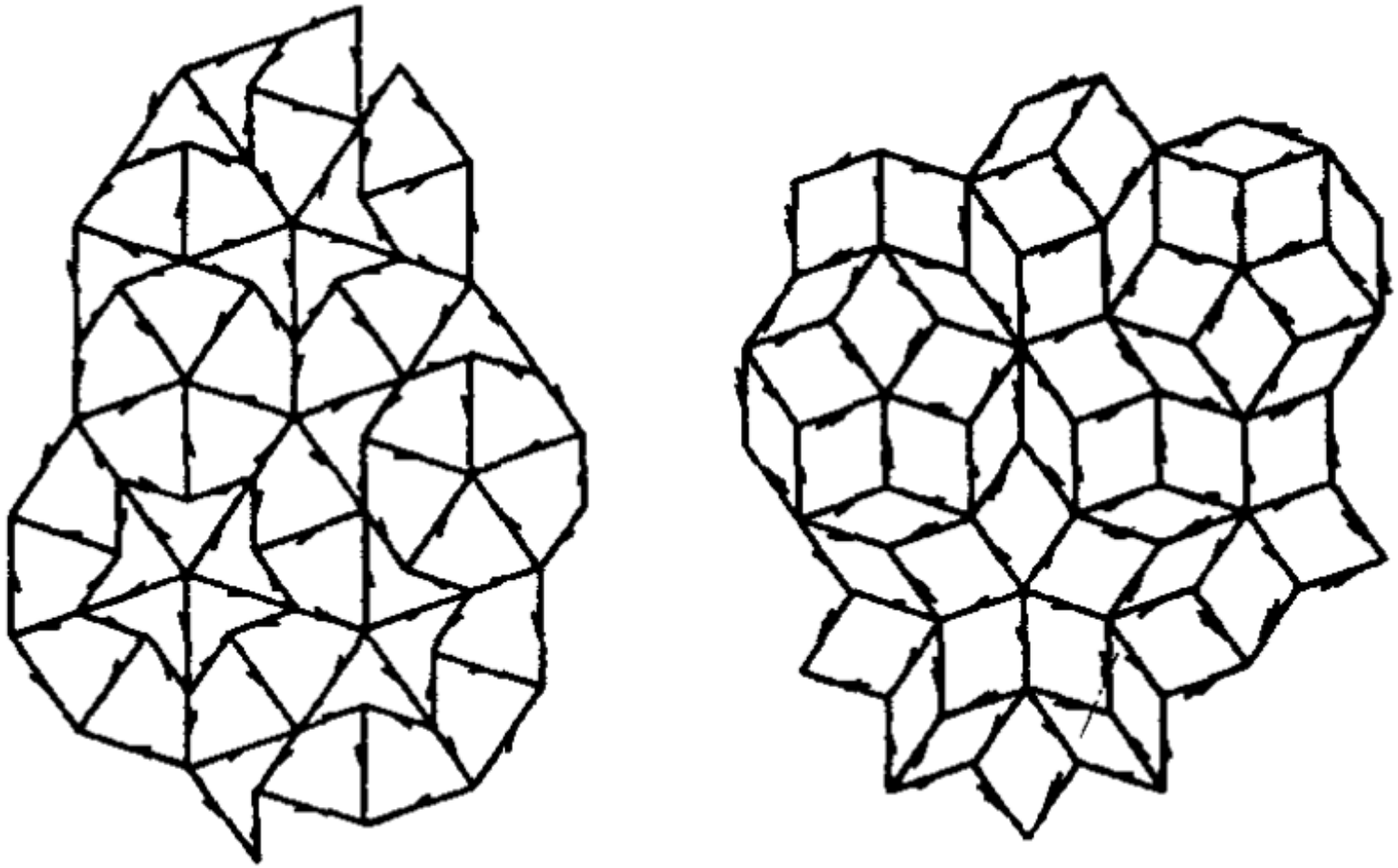
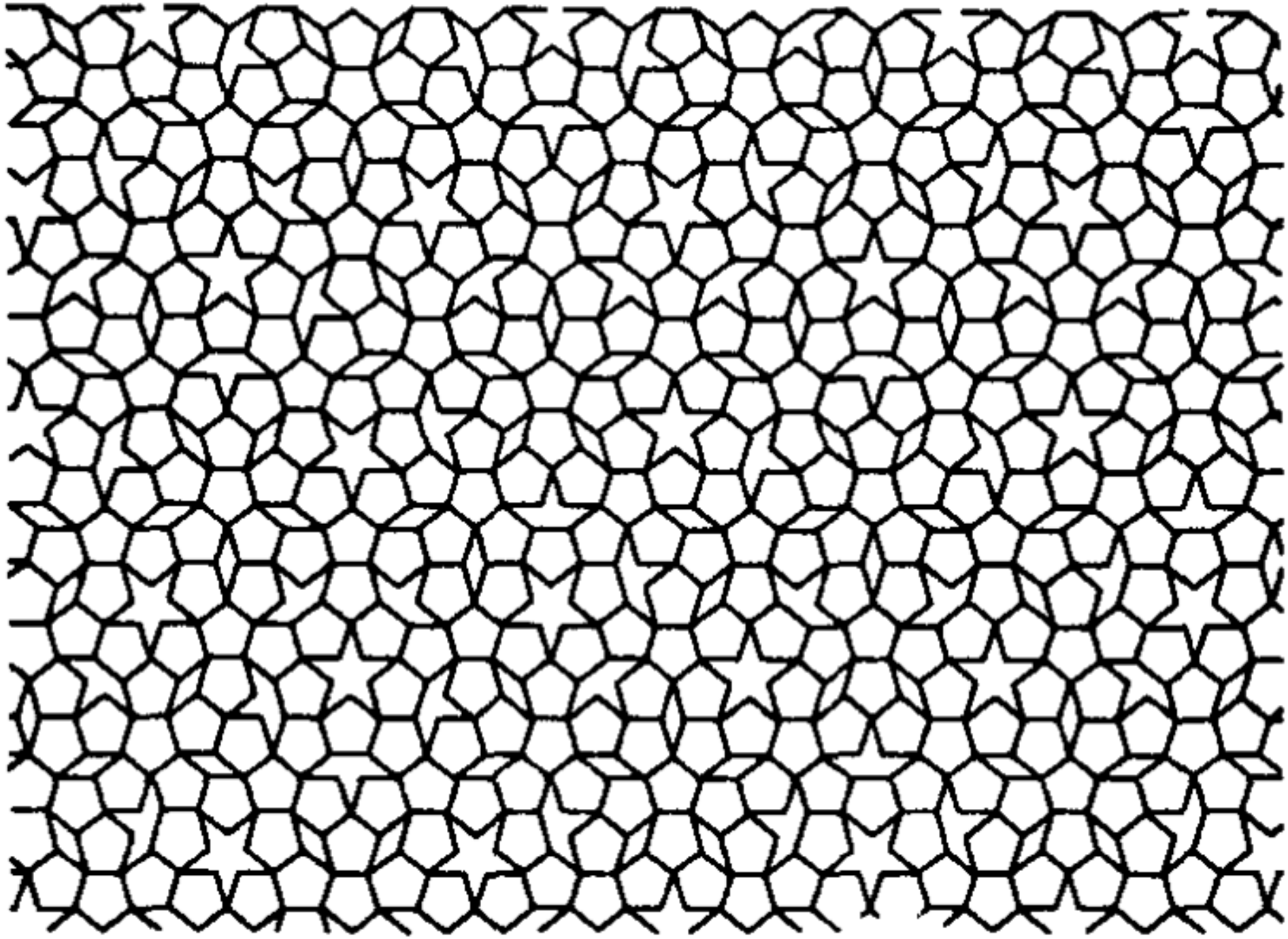


Рис. 4.12. Две пары плиток, которые покрывают плоскость только непериодически («плитки Пенроуза»). Также показано замощение плоскости каждой из этих пар



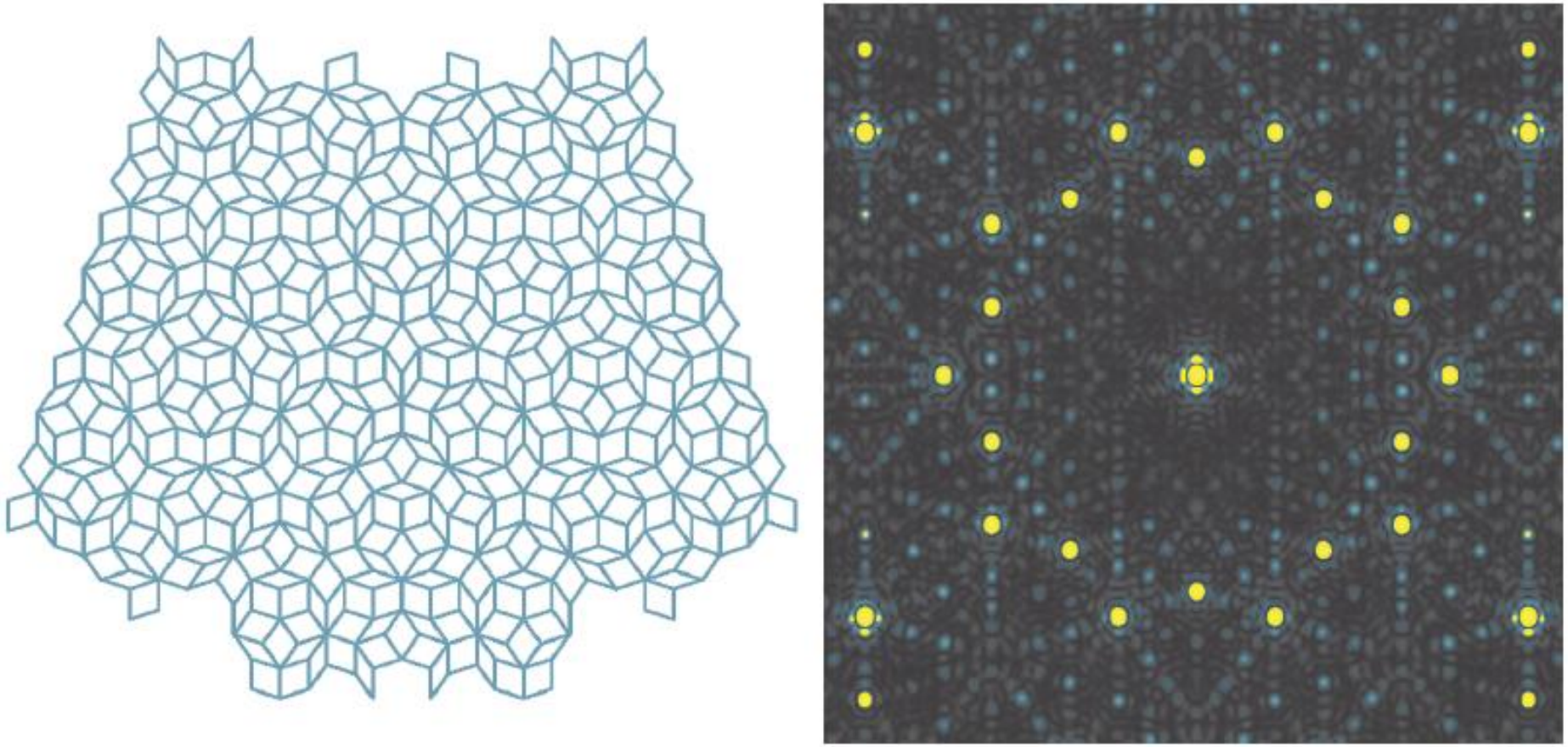
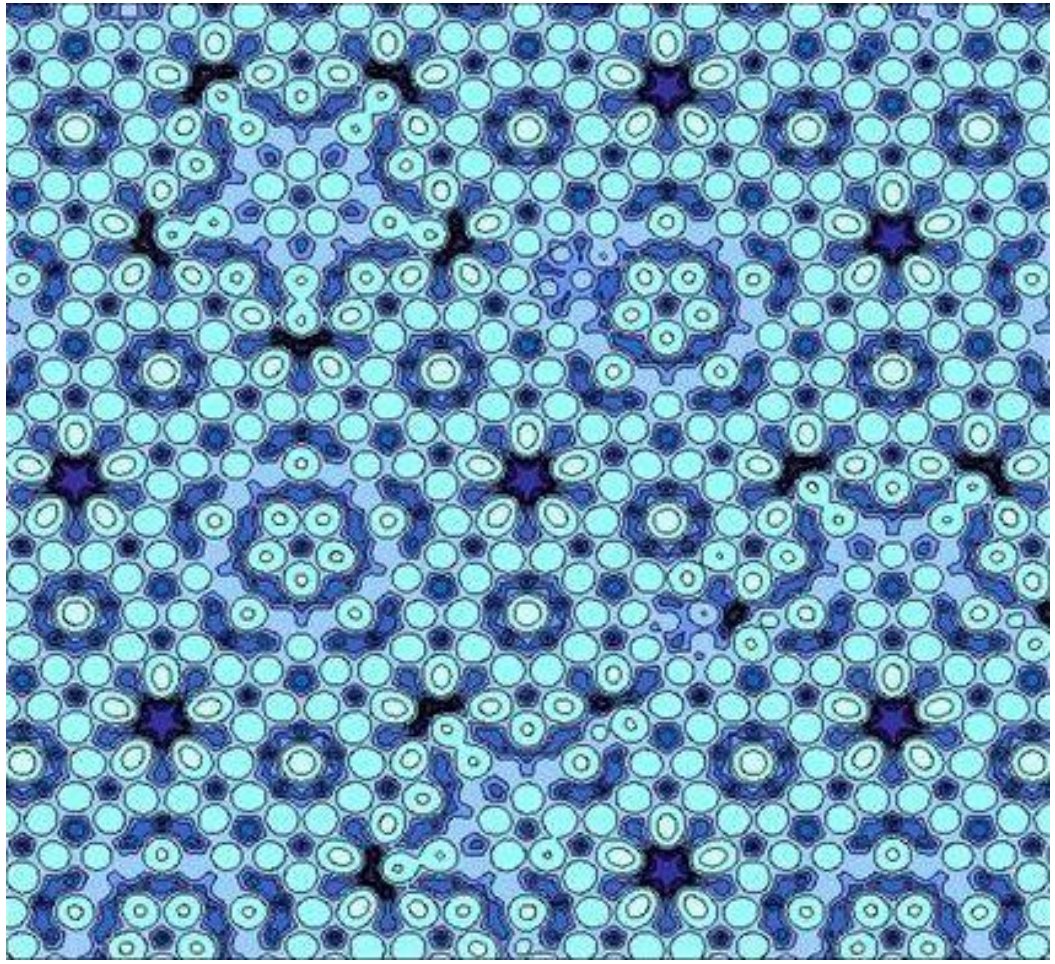
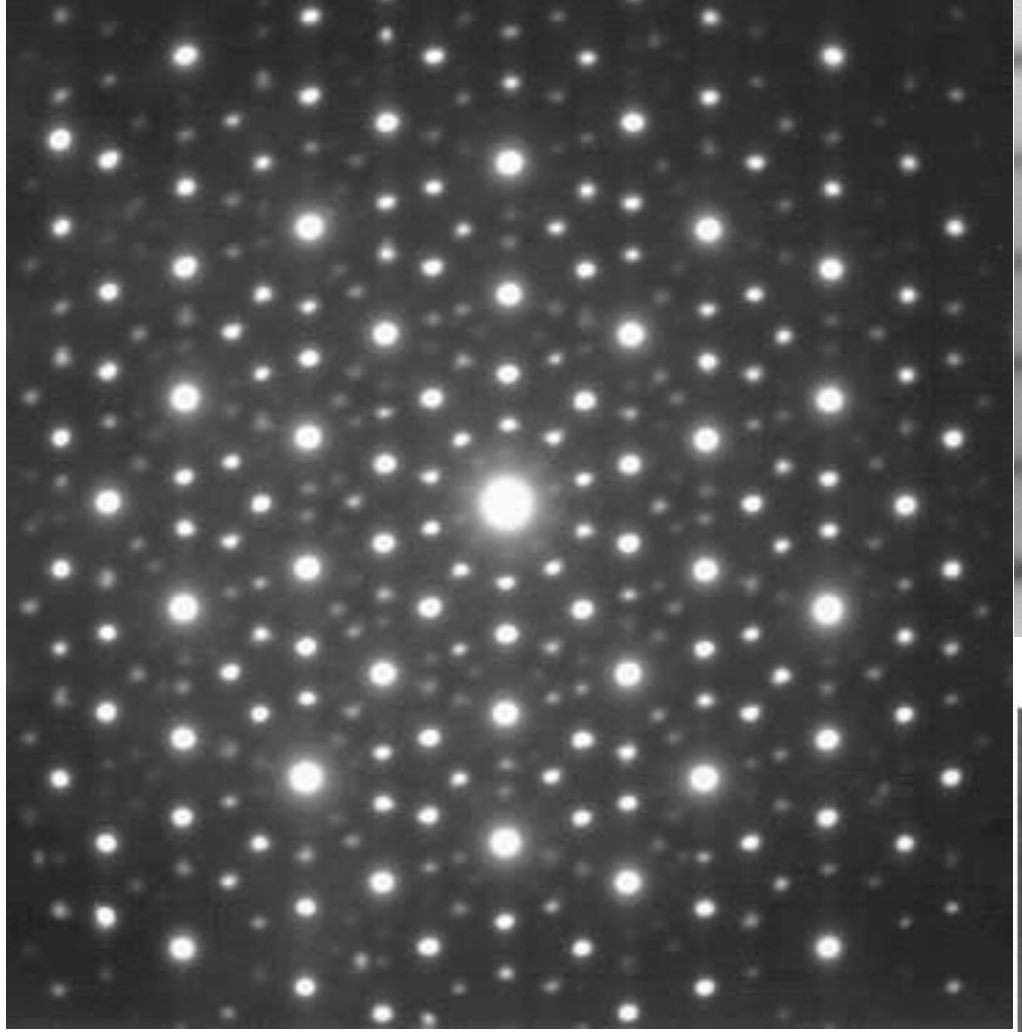
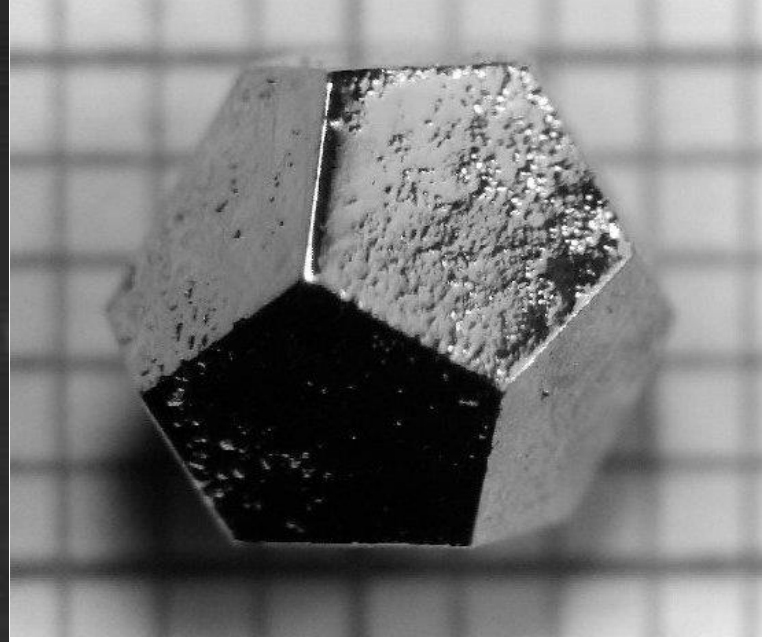


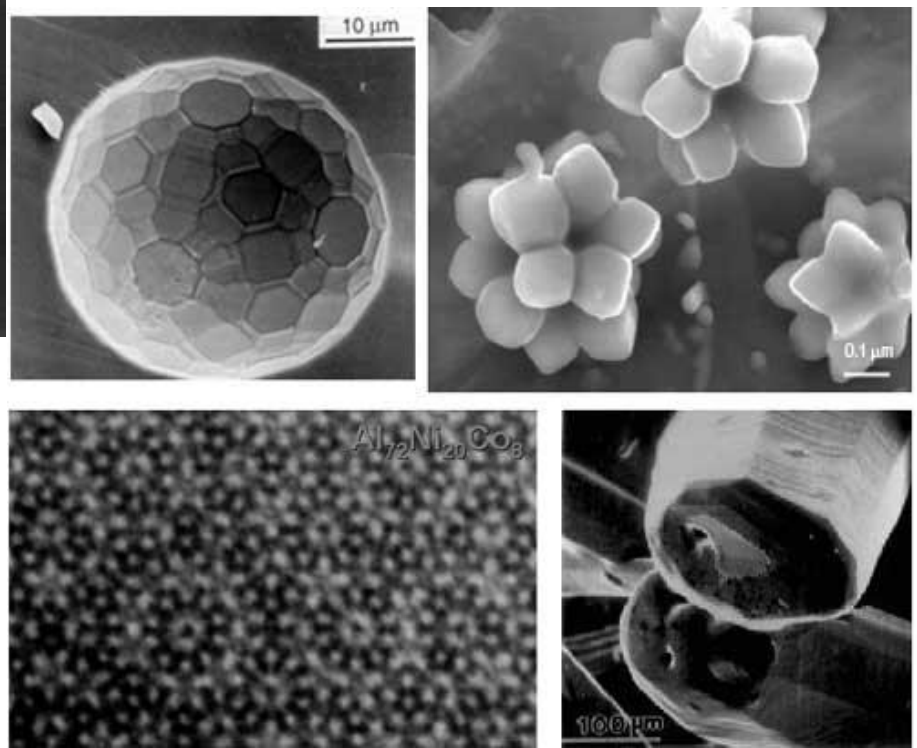
Figure 1. (a). A patch of a Penrose tiling. (b). The diffraction diagram of the vertex set V of (a) is essentially discrete; thus F is an aperiodic crystal, according to the new definition.



Atomic model of an aluminium-palladium-manganese (Al-Pd-Mn) quasicrystal surface.







Дифракційна картина розсіяння електонів на ікосаедричній структурі квазікристалу Zn-Mg-Ho. Видно 10 точок по колу.