Incommensurate charge density wave vector on multiband intermetallic systems

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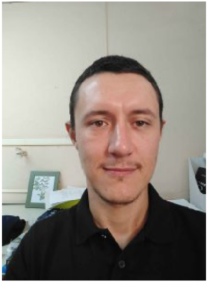

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Our results are discussed in these papers

PHYSICAL REVIEW B **107**, 205141 (2023)

Incommensurate charge density wave in multiband intermetallic systems exhibiting competing orders

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PHYSICAL REVIEW B **103**, 195150 (2021)

Interplay between charge density wave and superconductivity in multiband systems with interband Coulomb interaction

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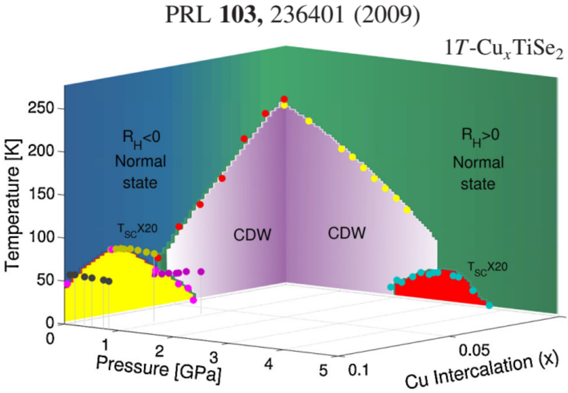
Overview

- Experimental motivation: charge density orders and superconductivity in transition - metal dichalcogenides (TMDs)
- Some previous theoretical works
- Hamiltonian model and formalism
- Results
- Conclusions

CDW x SC: Experimental motivation

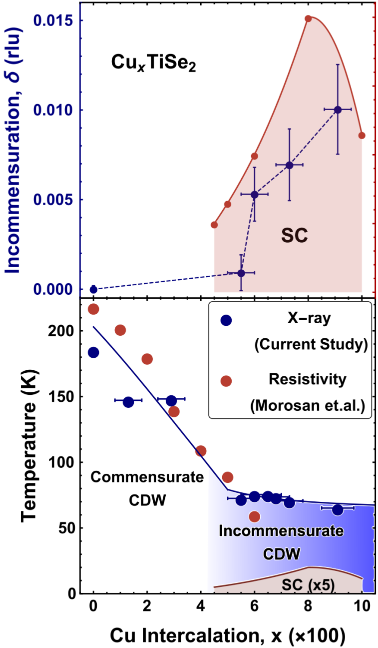
- Pressure and Cu intercalation induce superconductivity in pristine 1T-Cu_xTiSe_2



CDW - inCDW x SC: Experimental motivation

Observation of a charge density wave incommensuration near the superconducting dome in Cu_xTiSe_2

A. Kogar *et al.* Phys. Rev. Lett. **118**, 027002 (2017)



Some previous works

- Theoretical models considering electronic origin for CDW order, without superconductivity

PHYSICAL REVIEW B **72**, 125122 (2005)

Competing orderings in an extended Falicov-Kimball model

$$\mathcal{H} = -t\sum_{\langle i,j\rangle} d_i^\dagger d_j + \epsilon_f \sum_j n_j^f + \sum_{i,j} (V_{ij} d_i^\dagger f_j + \text{H.c.}) + U\sum_j n_j^d n_j^f.$$

PHYSICAL REVIEW B **77**, 155130 (2008)

Hartree-Fock study of electronic ferroelectricity in the Falicov-Kimball model with *f*-*f* hopping

$$H = -t_d \sum_{\langle ij\rangle} d_i^+ d_j - t_f \sum_{\langle ij\rangle} f_i^+ f_j + U\sum_i f_i^+ f_i d_i^+ d_i + E_f \sum_i f_i^+ f_i,$$

P. M. R. Brydon *et al.*, PRB **72**, 125122 (2005)

P. Farkasovsky PRB **77**, 155130 (2008)

Hamiltonian: two-band model and formalism (Our model generalizes previous works)

$$
\begin{aligned}
H = & - t_c \sum_{\langle ij \rangle, \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + \mathrm{H.c.}) - t_d \sum_{\langle ij \rangle, \sigma} (d^\dagger_{i\sigma} d_{j\sigma} + \mathrm{H.c.}) \\
& + \epsilon_{d0} \sum_{i,\sigma} d^\dagger_{i\sigma} d_{i\sigma} - \mu \sum_{i,\sigma} (d^\dagger_{i\sigma} d_{i\sigma} + c^\dagger_{i\sigma} c_{i\sigma}) \\
& + \sum_{i,\sigma} V_{ij} (c^\dagger_{i\sigma} d_{j\sigma} + d^\dagger_{i\sigma} c_{j\sigma}) \\
& + U_{dc} \sum_i n^d_i n^c_i + J_d \sum_i d^\dagger_{i\uparrow} d_{i\uparrow} d^\dagger_{i\downarrow} d_{i\downarrow} \ ,
\end{aligned}
$$

where $c_{i\sigma}$ ($c^\dagger_{i\sigma}$) and $d_{i\sigma}$ ($d^\dagger_{i\sigma}$) denote annihilation (creation) operators of c- and d-electrons, respectively, in a given site i, with spin σ, in the standard second quantization formalism.

Some parameters of the model

$$\langle n_i^c \rangle = n^c + \delta^c \cos(\mathbf{Q} \cdot \mathbf{R}_i),$$
$$\langle n_i^d \rangle = n^d + \delta^d \cos(\mathbf{Q} \cdot \mathbf{R}_i),$$

- δ^c and $\delta^d \rightarrow$ **CDW/inCDW order parameters**.

$$\delta^c = \frac{1}{N} \sum_{\mathbf{k}}{}' \Big(\langle c^\dagger_{\mathbf{k}+\mathbf{Q}\sigma} c_{\mathbf{k}\sigma} \rangle + \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}+\mathbf{Q}\sigma} \rangle \Big)$$

- $\mathbf{Q} = (Q_x, Q_y)$ is the modulation wave vector.
- **Considering non-magnetic state**

$$\langle n_\uparrow^{d(c)} \rangle = \langle n_\downarrow^{d(c)} \rangle.$$

- **Superconducting order parameter**

$$\Delta^d_{\mathbf{k}} \equiv J_d \langle d_{-\mathbf{k}\downarrow} d_{\mathbf{k}\uparrow} \rangle$$

The matrix Hamiltonian

$H_{MF} = \sum_{\mathbf{k}}{}' \Psi^\dagger_{\mathbf{k}} M \Psi_{\mathbf{k}} + \mathcal{C}$, using the Nambu's spinor basis,

$$\Psi^\dagger = \left(c^\dagger_{\mathbf{k}\uparrow}, c^\dagger_{\mathbf{k+Q}\uparrow}, d^\dagger_{\mathbf{k}\uparrow}, d^\dagger_{\mathbf{k+Q}\uparrow}, c_{-\mathbf{k}\downarrow}, c_{-\mathbf{k-Q}\downarrow}, d_{-\mathbf{k}\downarrow}, d_{-\mathbf{k-Q}\downarrow} \right) \;,$$

$M =$

$$\begin{pmatrix}
\epsilon^c_{\mathbf{k}} & U_{dc}\delta^d & V_{\mathbf{k}} & 0 & 0 & 0 & 0 & 0 \\
U_{dc}\delta^d & \epsilon^c_{\mathbf{k+Q}} & 0 & V_{\mathbf{k+Q}} & 0 & 0 & 0 & 0 \\
V^*_{\mathbf{k}} & 0 & \epsilon^d_{\mathbf{k}} & U_{dc}\delta^c & 0 & 0 & \Delta^d_{\mathbf{k}} & 0 \\
0 & V^*_{\mathbf{k+Q}} & U_{dc}\delta^c & \epsilon^d_{\mathbf{k+Q}} & 0 & 0 & 0 & \Delta^d_{\mathbf{k+Q}} \\
0 & 0 & 0 & 0 & -\epsilon^c_{-\mathbf{k}} & -U_{dc}\delta^d & -V^*_{-\mathbf{k}} & 0 \\
0 & 0 & 0 & 0 & -U_{dc}\delta^d & -\epsilon^c_{-\mathbf{k-Q}} & 0 & -V^*_{-\mathbf{k-Q}} \\
0 & 0 & \Delta^{d*}_{-\mathbf{k}} & 0 & -V_{-\mathbf{k}} & 0 & -\epsilon^d_{-\mathbf{k}} & -U_{dc}\delta^c \\
0 & 0 & 0 & \Delta^{d*}_{-\mathbf{k-Q}} & 0 & -V_{-\mathbf{k-Q}} & -U_{dc}\delta^c & -\epsilon^d_{-\mathbf{k-Q}}
\end{pmatrix}$$

$\epsilon_{\mathbf{k}} = -2t_c\left[\cos(k_x a) + \cos(k_y a)\right]$, $\epsilon^c_{\mathbf{k}} \equiv \epsilon_{\mathbf{k}} + U_{dc}n^d - \mu$,
$\epsilon^d_{\mathbf{k}} \equiv \gamma\epsilon_{\mathbf{k}} + U_{dc}n^c - \mu + \epsilon_{d0}$, $\gamma = t_d/t_c$
ϵ_{d0} is the relative depth between the centers of the bands.

Bogoliubov - de Gennes transformation

$$H_{\text{diag}} = \sum_{\mathbf{k}}{}' \sum_{m=1,2,3,4} E_{m\mathbf{k}} \left(\alpha^{\dagger}_{m\mathbf{k}} \alpha_{m\mathbf{k}} + \beta^{\dagger}_{m\mathbf{k}} \beta_{m\mathbf{k}} \right) + \mathcal{C} \,,$$

where $(\alpha, \beta)^{\dagger}_{m\mathbf{k}}$ and $(\alpha, \beta)_{m\mathbf{k}}$ are new operators given by a linear combination of the original band operators $(c, d)^{\dagger}$ and (c, d).
The free energy density is calculated as follows

$$F = -2T \sum_{\mathbf{k}}{}' \sum_{m} \ln \left[1 + \exp \left(-\beta E_{m\mathbf{k}} \right) \right] + \mathcal{C},$$

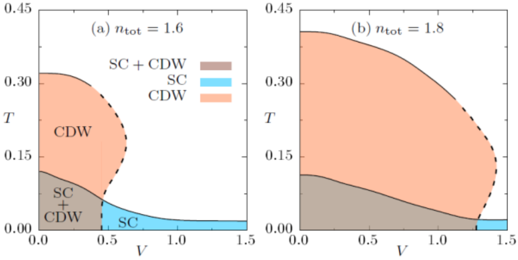
where $\beta = 1/(k_B T)$. We emphasize that we consider both incommensurate and commensurate periodic modulations of the crystal lattice with $\mathbf{Q} = (Q_x, Q_y)$.

$$\frac{\partial F}{\partial \mu} = \frac{\partial F}{\partial n^d} = \frac{\partial F}{\partial \delta^d} = \frac{\partial F}{\partial \delta^c} = \frac{\partial F}{\partial \Delta^d} = \frac{\partial F}{\partial Q_x} = \frac{\partial F}{\partial Q_y} = 0.$$

Commensurate modulation: $\mathrm{Q} = (\frac{\pi}{a}, \frac{\pi}{a})$

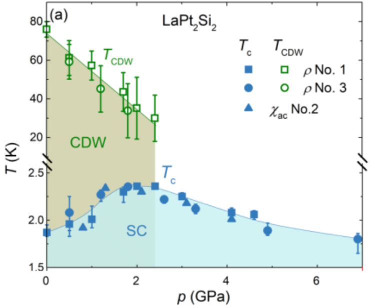
- Comparing our results with an experimental phase diagram

Physical Review B **103**, 195150 (2021)



$U_{dc} = 1.2$, $J_d = -1.0$, and $\epsilon_{d0} = 0.0$.

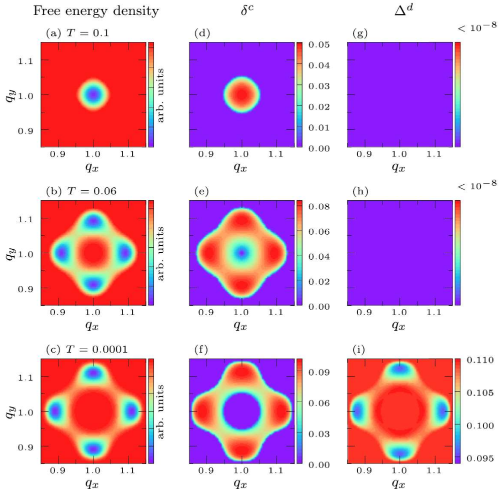
PHYSICAL REVIEW B **101**, 144501 (2020)



NL, **DR**, MC, CT, PRB **103**, 195150 (2021)

Results

Is the stable solution a mixing phase for SC + inCDW?



$n_{\text{tot}} = 1.6,\ V = 0.5,\ J = -1.0,$
$\epsilon_{d0} = 0.0,\ U_{dc} = 1.2$

$$q_x = Q_x/\pi$$

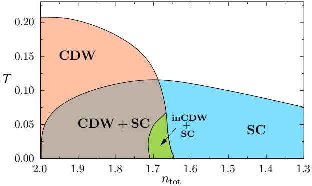
$$q_y = Q_y/\pi$$

For inCDW

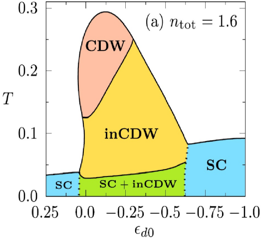
$$\mathbf{Q} = (Q_x, \pi) \equiv (\pi, Q_y)$$

Results

$T \times n_{tot}$ and $T \times \epsilon_{d0}$ phase diagram



$J = -1.0,\ U_{dc} = 0.8,\ V = 0.0,\ \epsilon_{d0} = 0.0$



$J = -1.0,\ U_{dc} = 1.2,\ V = 0.5$

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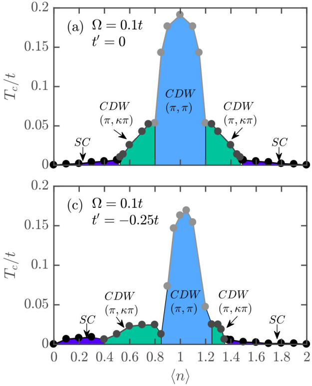

Comparing with one band model interacting via e-ph. P.M. Dee *et al.* PRB **99**, 024514 (2019)

Conclusions

- After analyzing the free energy density, we discovered that under certain parameter conditions, an incommensurate CDW emerges at low temperatures and can coexist with superconductivity.
- Away from half-filling, our findings align qualitatively with previously reported results observed in compounds that undergo a discontinuous disappearance of the CDW transition, indicating a first-order phase transition.
- Besides these findings, we have obtained diverse phase diagrams using our model. For instance, hybridization and Coulomb repulsion as a function of band filling, among others.