ISTITUTO ITALIANO DI TECNOLOGIA

SCUOLA NORMALE SUPERIORE

Interacting orders in functional materials

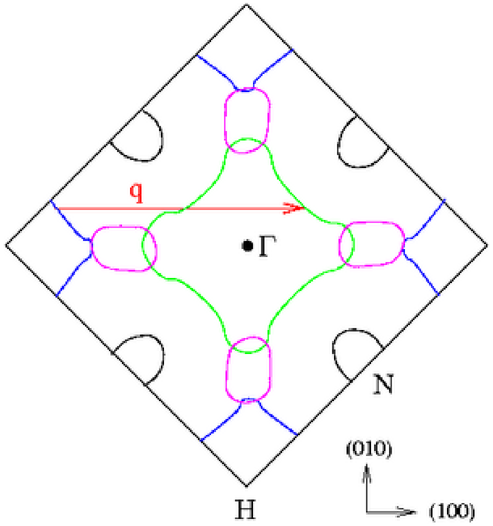
Louis Ponet

Cr: charge and spin density wave, and ultrafast control

- Fermi surface nesting: High T_N spin density wave (311 K)
- Exchange striction → charge density wave

$$H = \sum_{<i,j>} J(r_{i,j}) \boldsymbol{S}_i \boldsymbol{S}_j; \qquad r_{i,j} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$$

$$J(r_{i,j}) = J(r_{i,j}^0) + \left.\frac{dJ}{dr_{i,j}}\right|_{r=r^0} \delta r$$



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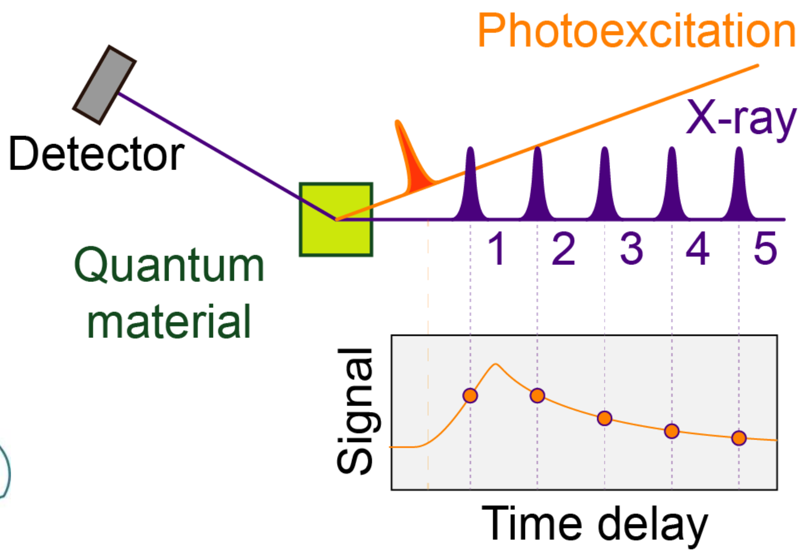
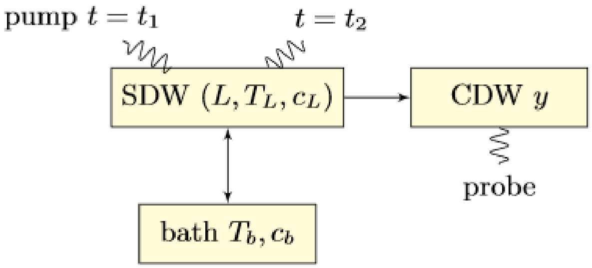
Cr: experimental setup

- Two optical pump pulses (40 fs width, 1-2 ps between pulses)
- x-ray probe monitors strain wave/CDW, created by SDW

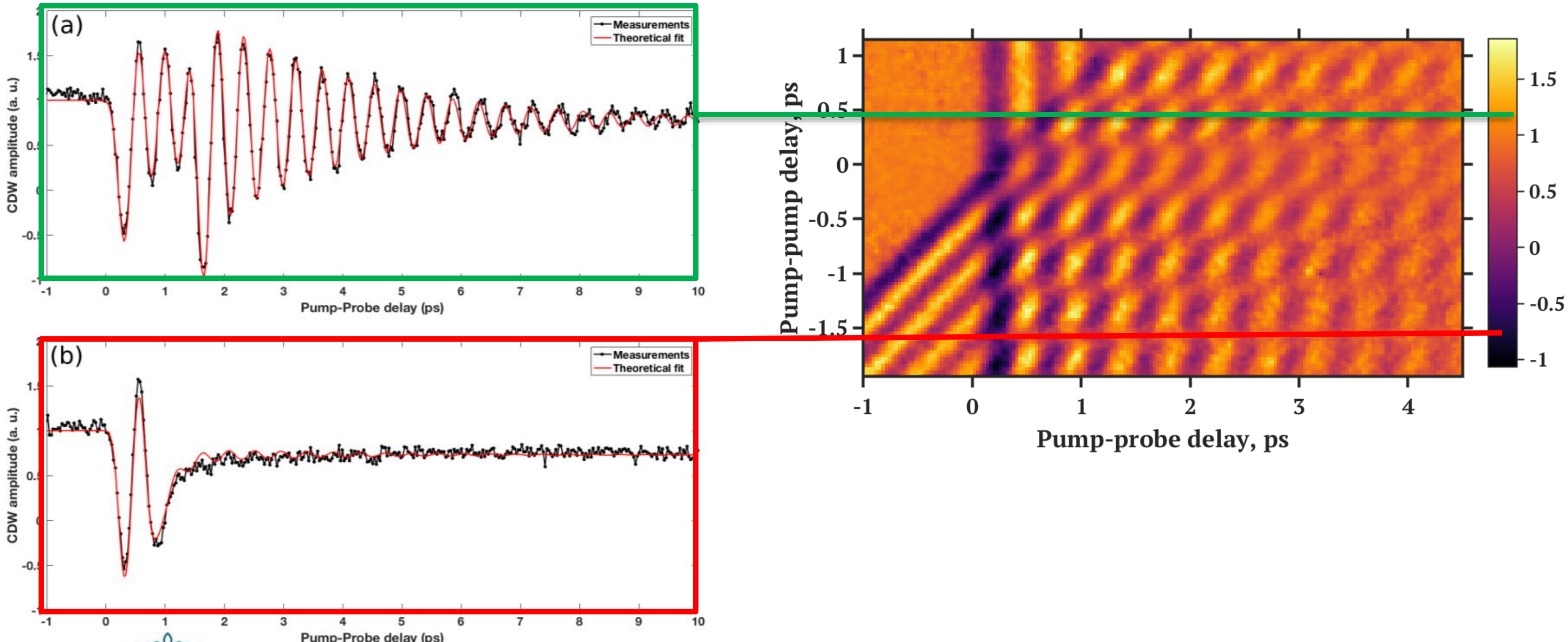
- Pulses heat up SDW
- Electrostriction → CDW amplitude oscillations





Cr: experimental results

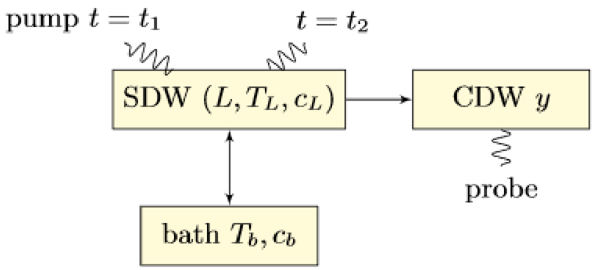
- 2 pulses: Constructive or destructive interference



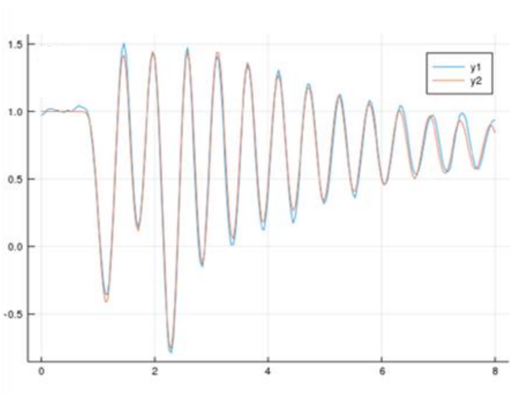
Measurements performed by group of Prof. Singer A. at Cornell University

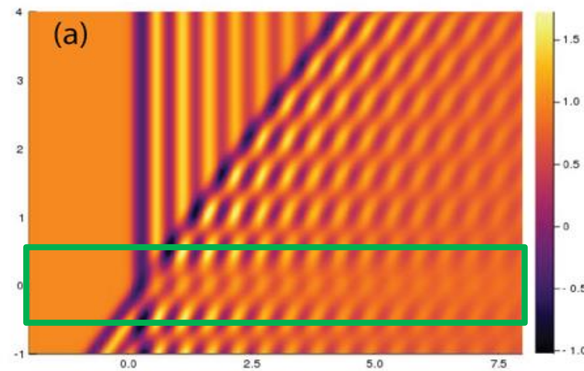
Cr: theory

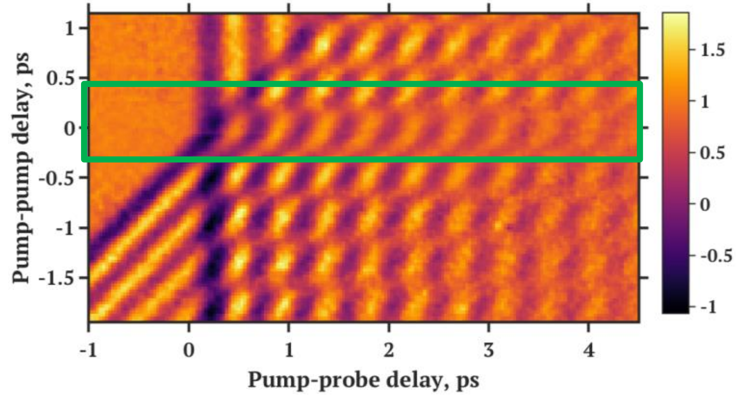
- CDW ⇔ SDW, 1st order transition
- Two order parameters: L, y
- $F = \frac{\alpha}{2}(T_L - T_c)L^2 + \frac{\beta_L}{4}L^4 - gL^2y + \frac{\omega^2}{2}y^2 + \frac{\beta_y}{4}y^4$
- Two temperatures: T_b, T_L
- Pulses applied to T_L

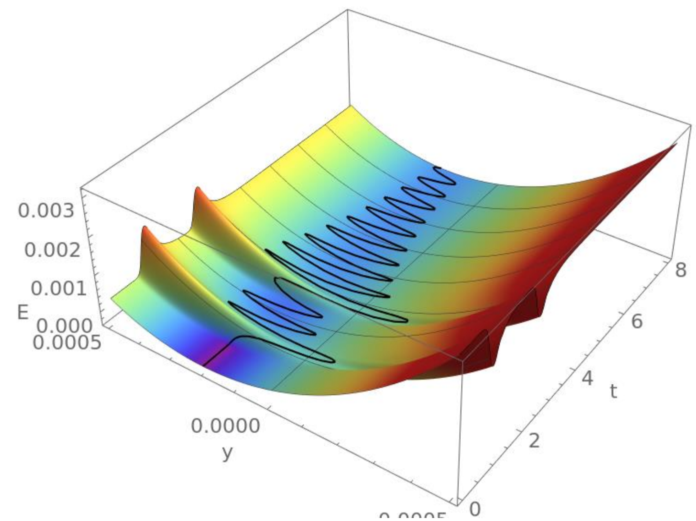


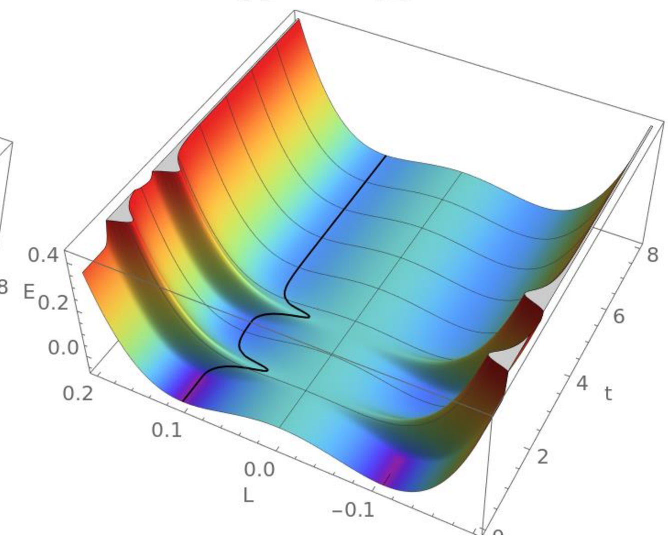
Cr: theoretical results











$$F_y = -gL^2 y + \frac{\omega^2}{2} y^2 + \frac{\beta_y}{4} y^4 \qquad F_L = \frac{\alpha}{2}(T_L - T_c)L^2 + \frac{\beta_L}{4} L^4 - gL^2 y$$

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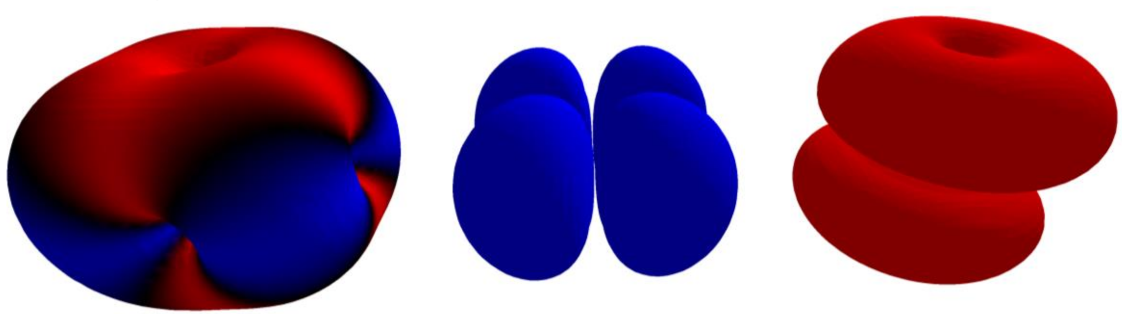
Magnetism

- Interaction between spin order and orbital order in high spin-orbit coupled materials
- Heavy ions, e.g. Sr2IrO4, NaIrO3
- $\lambda\, \boldsymbol{l} \cdot \boldsymbol{S}\, ;\, \lambda \sim Z^2$
- $\boldsymbol{S} \rightarrow \tilde{\boldsymbol{S}}$

$$\left|\tilde{\uparrow}\right\rangle = sin(\theta)\left|0,\uparrow\right\rangle - cos(\theta)\left|+1,\downarrow\right\rangle$$

$$\left|\tilde{\downarrow}\right\rangle = sin(\theta)\left|0,\downarrow\right\rangle - cos(\theta)\left|-1,\uparrow\right\rangle$$

$$\left|\tilde{\uparrow}\right\rangle \;=\; \left|0,\uparrow\right\rangle \;+\; \left|1,\downarrow\right\rangle$$



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Model

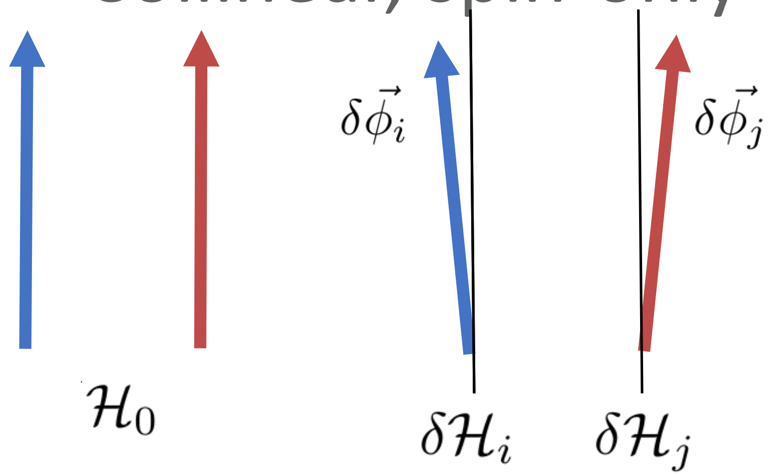
- Extended Heisenberg Hamiltonian

$$H = \sum_{<ij>} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \quad \Rightarrow \quad \mathcal{H}_{exch} = \sum_{i,j} \vec{m}_i \mathcal{J}_{ij} \vec{m}_j$$

- Includes terms like Kitaev exchange

Numerical Calculation

- Based on Green's functions
- Collinear, spin-only case (purely isotropic):



$$\delta\mathcal{H}_i = 1/2 i \delta\vec{\phi}_i [\mathcal{H}_i, \vec{\sigma}_i]$$

$$\Delta_i = \mathcal{H}_i^{\uparrow\uparrow} - \mathcal{H}_i^{\downarrow\downarrow}$$

$$\delta\mathcal{H}_i = \frac{\Delta_i}{2}\left(\delta\phi_i^y \sigma_i^x - \delta\phi_i^x \sigma_i^y\right)$$

$$J_{ij} = \frac{1}{4\pi}\int_{-\infty}^{E_f} d\epsilon \, Sp \, Im \left[\Delta_i G_{ij}^{\downarrow} \Delta_j G_{ji}^{\uparrow}\right]$$

KKR: A.I. Liechtenstein et al. Journal of Magnetism and Magnetic Materials (1987), *67*, 65–74.
LDA+U: V. V. Mazurenko, *Phys. Rev. B, 71*(18), 1–8, *(2005)*, .
LDA+U & Wannier90: D. M. Korotin, Phys. Rev. B (91), *224405*, 1–7 (2015).

Numerical Calculation

- SOC case:
  - σ is not a good quantum number → j
  - Spins might be noncolinear → local z-axis changes
  - Rotation of j rotates charge, changes hopping, G
  - Lot bigger space to rotate in $\delta\mathcal{H}_i = 1/2i\delta\vec{\phi}_i[\mathcal{H}_i, \vec{j}_i]$
- Solution: rotate effective on-site $\boldsymbol{B}$ field

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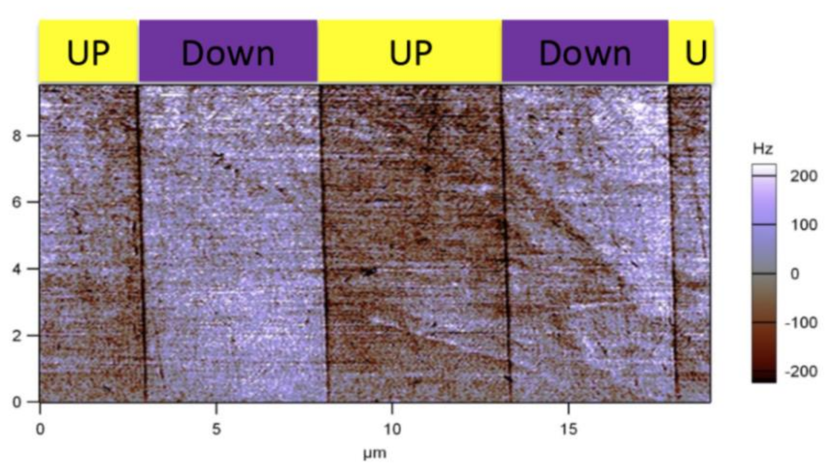
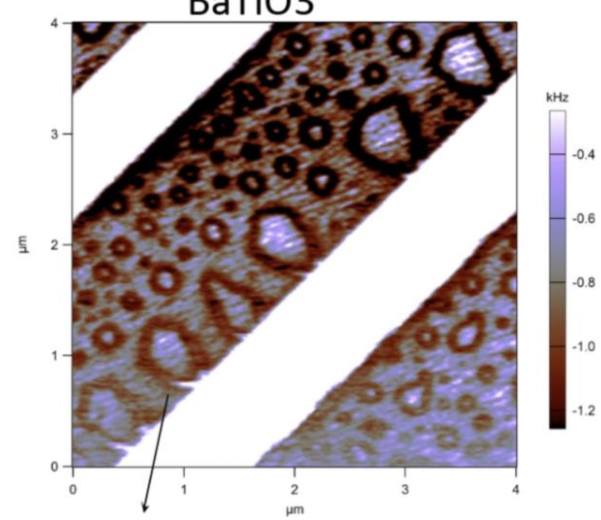
Domain wall-induced elastic softening

- Interaction between ferroelectric polarization and strains
  - Apparent mechanical softening





Measurement performed by group of Prof. Catalan G. in Barcelona

Model

- Interaction with Structural order
- Model: Ginzburg-Landau-Devonshire

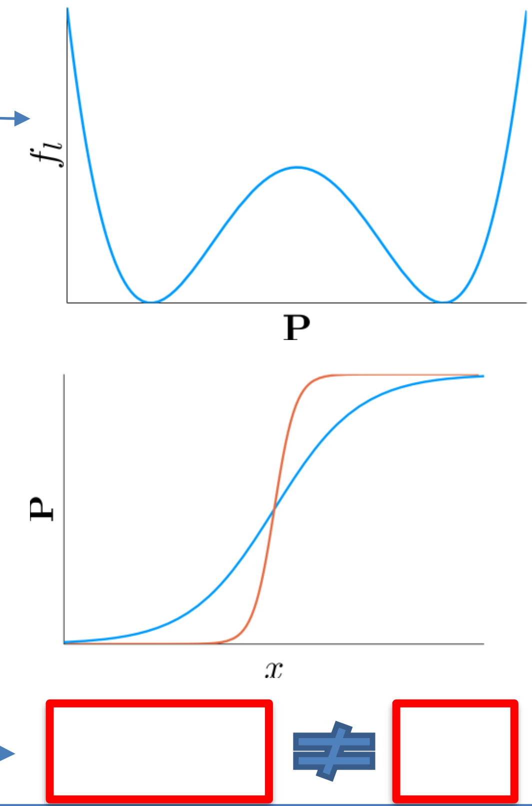
$$f_l = \alpha P^2 + \beta P^4 + \gamma P^6$$

$$f_g = G(\nabla P)^2$$

$$f_{es} = -qP^2\varepsilon$$

$$f_{el} = C\varepsilon^2$$

$$f_{fl} = f(\nabla P\varepsilon + P\nabla\varepsilon)$$



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Model

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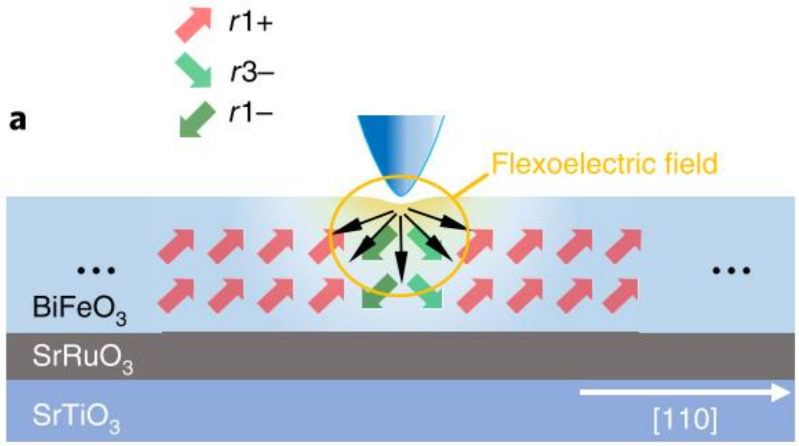
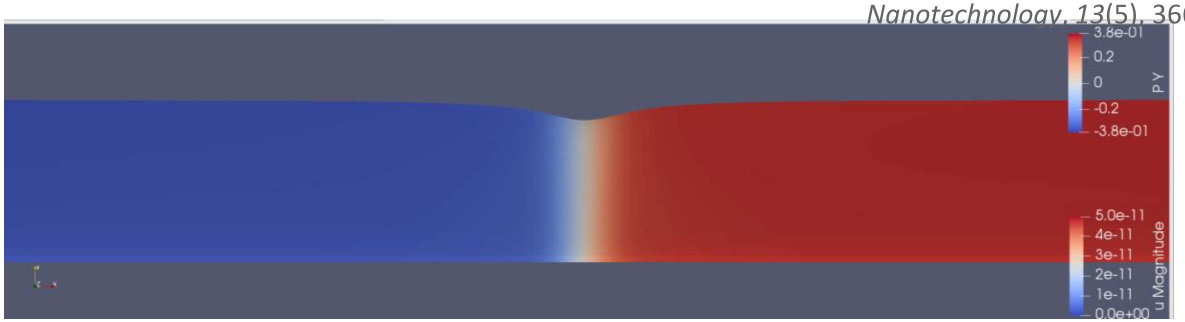


Park, S. M. et al, (2018). *Nature Nanotechnology*, *13*(5), 366–370.



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Simulations

- Finite element method

  - softness: $C_{eff} = \frac{\delta u}{\delta F}$