Ultrafast magnetic phase transition in $DyFeO_3$

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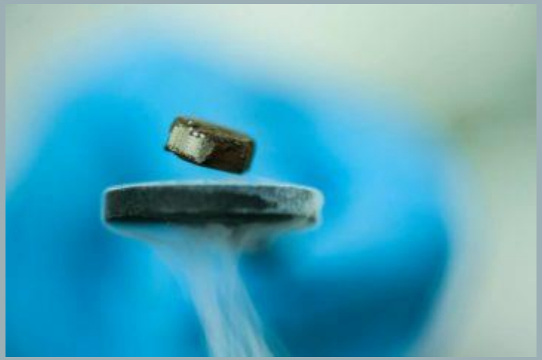
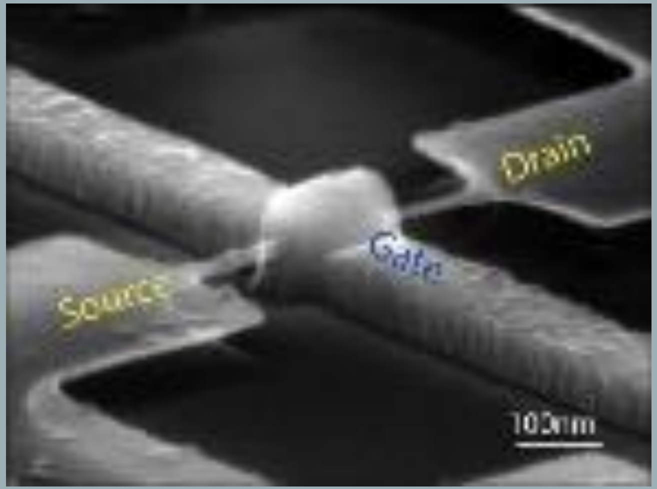
Introduction

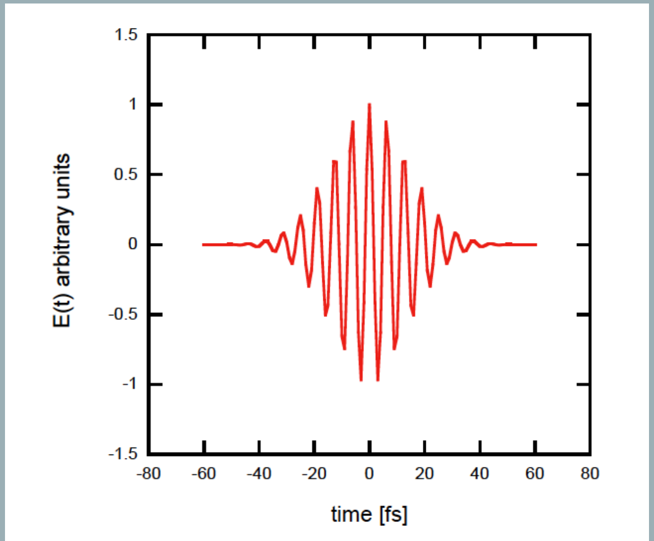


Improving the current technology by:

- ❑ New phenomena and new technology
- ❑ Miniaturization
- ❑ Device performance speed
  Using ultrafast laser pulses



Introduction to Ultrafast laser



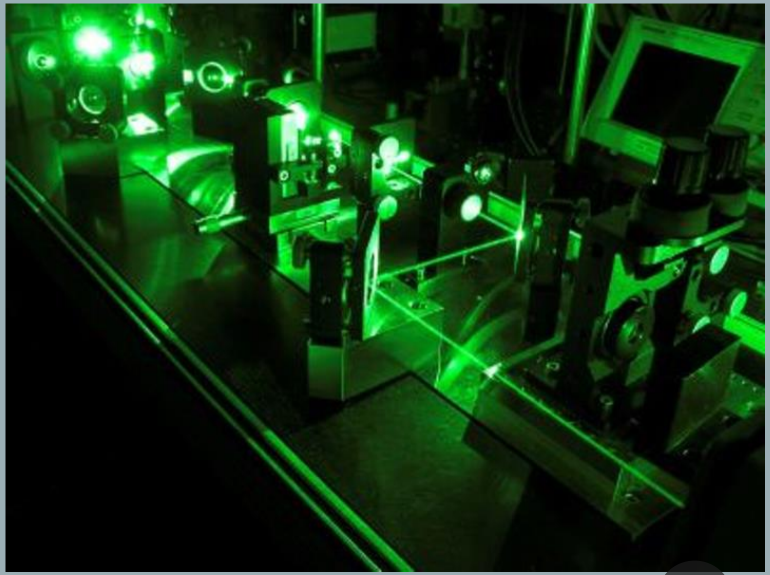
Ultrafast laser pulses?

Using ultrafast laser pulses to :

1. Study and understand Phenomena at ultrafast time scales

2. Change material properties

- ✓ Enhance superconductivity
- ✓ Switch ferroelectric polarization
- ✓ Induce ultrafast insulator-to-metal transitions
- ? Induce magnetic phase transition

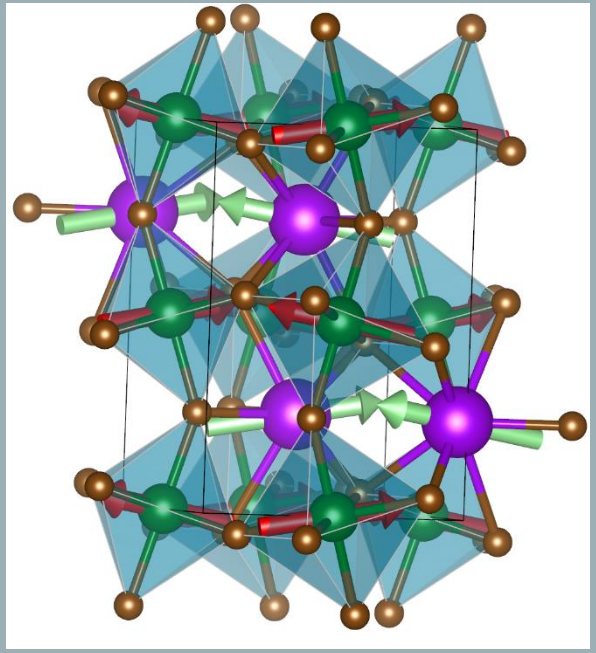


Material and laser

- Goal: Tuning magnetic phase transition in $DyFeO_3$ using ultrafast laser

- The laser has a 200 femtosecond impulsive source (with electric field of 10 MV cm^{-1})

- $DyFeO_3$: single crystal (Pnma phase)



$DyFeO_3$ magnetic properties

DyFeO3 has:

two stable magnetic phases:

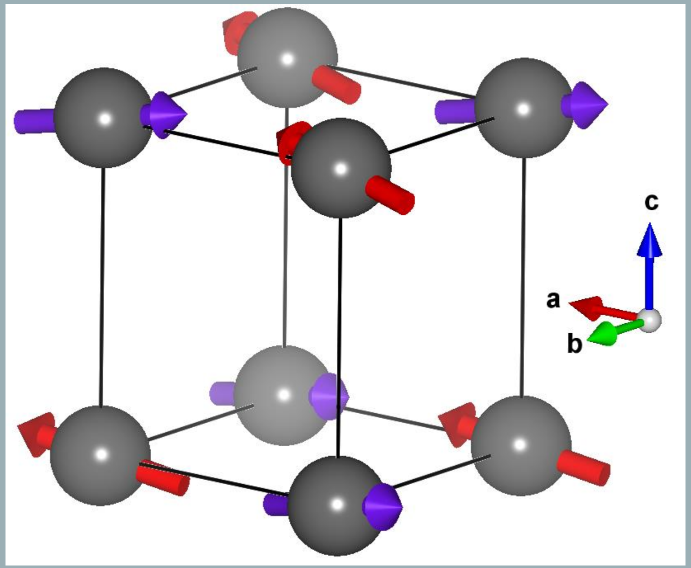
$T_N(Fe) = 650$ K vs $T_N(Dy) = 4.5$ K

Γ_4 $(G_xA_yF_z)$ at $T > 51$ K (weak ferromagnet)

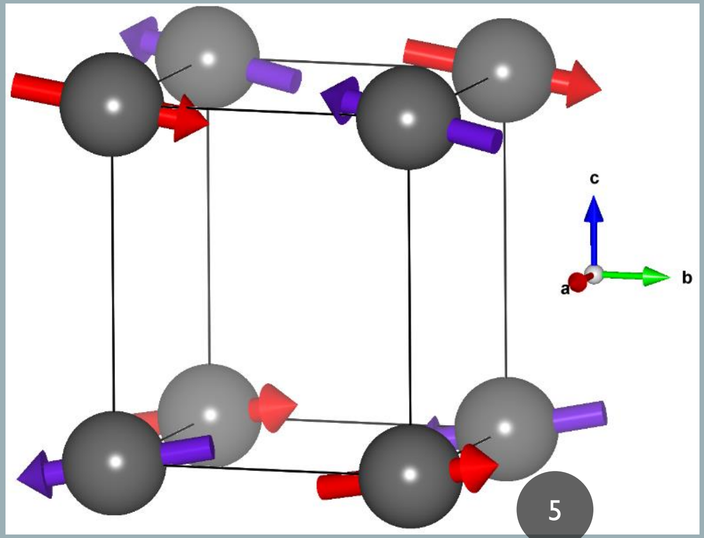
Γ_1 $(A_xG_yC_z)$ at $T < 51$ K

Fast magnetic phase transition at 51 K

Γ_4



Γ_1



Heisenberg model and DFT calculations

$$H = \sum_{ij} J_{ij} S_i S_j + \sum_{ij} D_{ij}.(S_i \times S_j) + \sum_i K_i (S_i.n_i)^2$$

J_{ij} → J_{MM} , J_{RM} Super exchange interactions

D_{ij} → D_{MM} , D_{RM} Dzyaloshinskii-Moriya interactions (DMI)

$D_{ij} = d_x^{ij} + d_y^{ij} + d_z^{ij}$ Is defined as DMI vector

K_i → K_M , K_R Single ion anisotropy

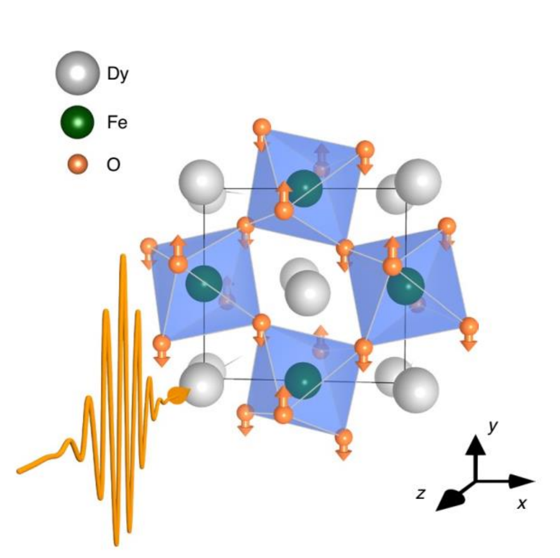
M = Fe and R=Dy

Phase transition is due to Dy and Fe interaction

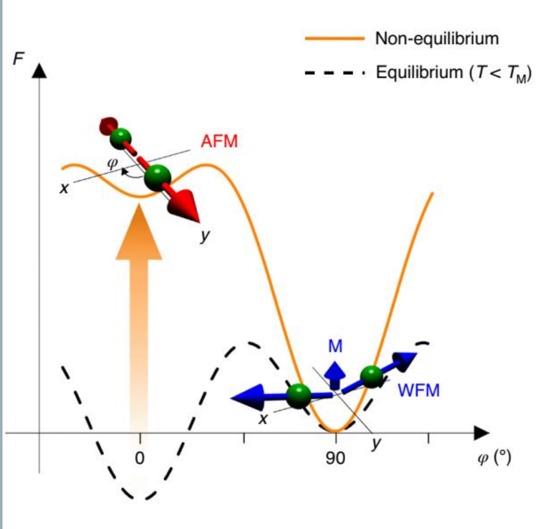
Sasani et al, arXiv:2102.08152 [cond-mat.mtrl-sci].

Experiment:

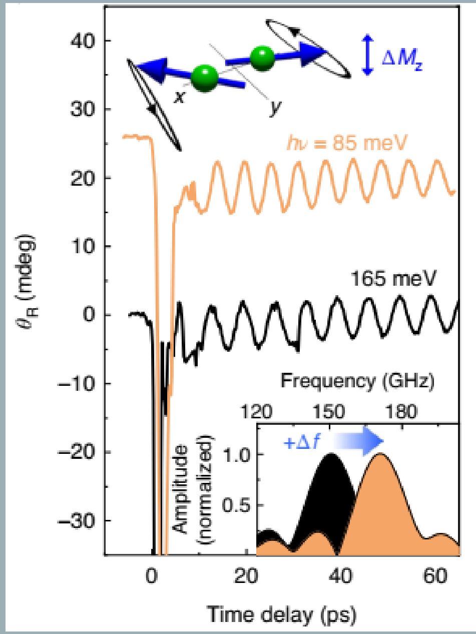
1. Ultra fast Laser field excites the high frequency IR Phonon modes

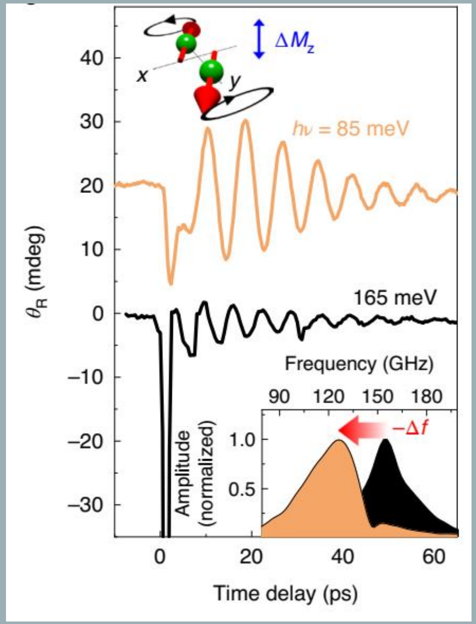


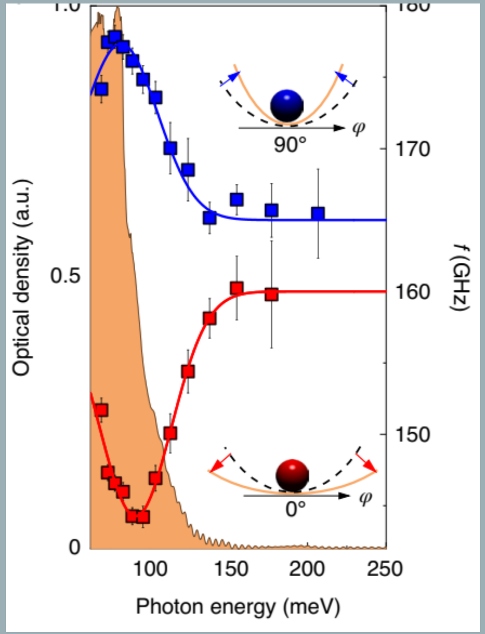
2. Excitation of phonons changes the magnetic potential energy surface



Experiment







Blue shift of magnon in Γ_4

Red shift of magnon in Γ_1

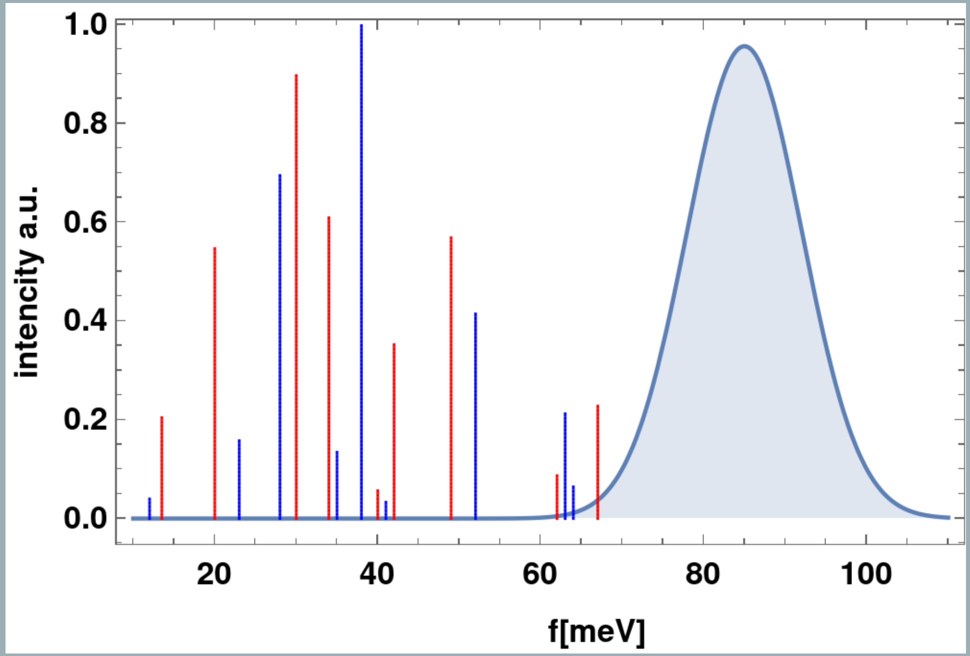
Red shift of magnon in Γ_1
Blue shift of magnon in Γ_4

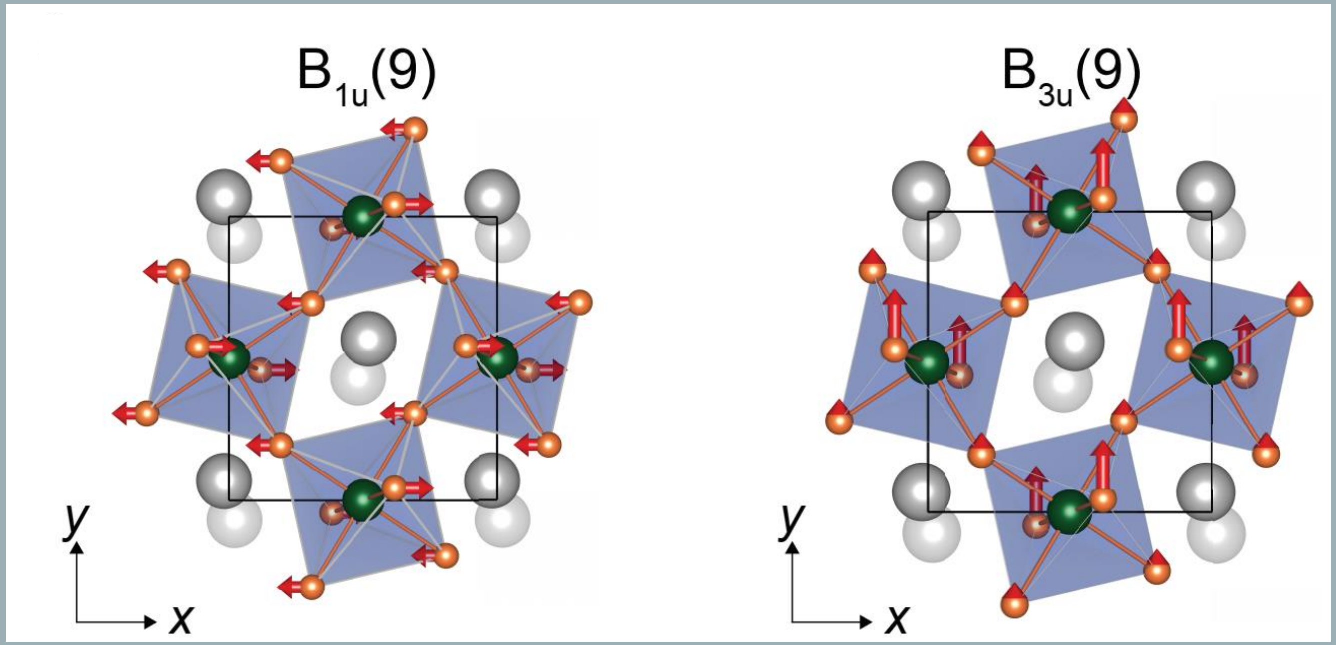
What is the mechanism behind this behaviour?

Technical details

- Density Functional Theory
- Projected Augmented Wave
- f electrons in the valence
- DFT+U (U=5 for Fe and U=4 for Dy)
- Occupation matrix constraint to find electronic ground state of Dy-f
- To calculate magnetic interaction we used Green's function method using TB2J code

Phonons excitation





Phonon modes and laser $$E(\omega) = \frac{E_0}{2\pi\sigma_\omega} e^{\frac{-(\omega-\omega_0)^2}{2\sigma_\omega}}$$

Modes that couple to laser

- ❑ Excitation of high frequency IR modes cannot create magnetic phase transition by themselves
- ❑ Experiment : oscillation with lower frequency

Non linear phononics

- ❑ Excitation of IR active mode can couple to other modes non-linearly in particular to Raman active modes :

$$V(Q) = \omega_{IR}^2 Q_{IR}^2 + \omega_R^2 Q_R^2 + C_R Q_R^3 + \gamma_1 Q_R Q_{IR}^2 + \frac{1}{4} d_{IR} Q_{IR}^4 + \frac{1}{4} d_R Q_R^4$$

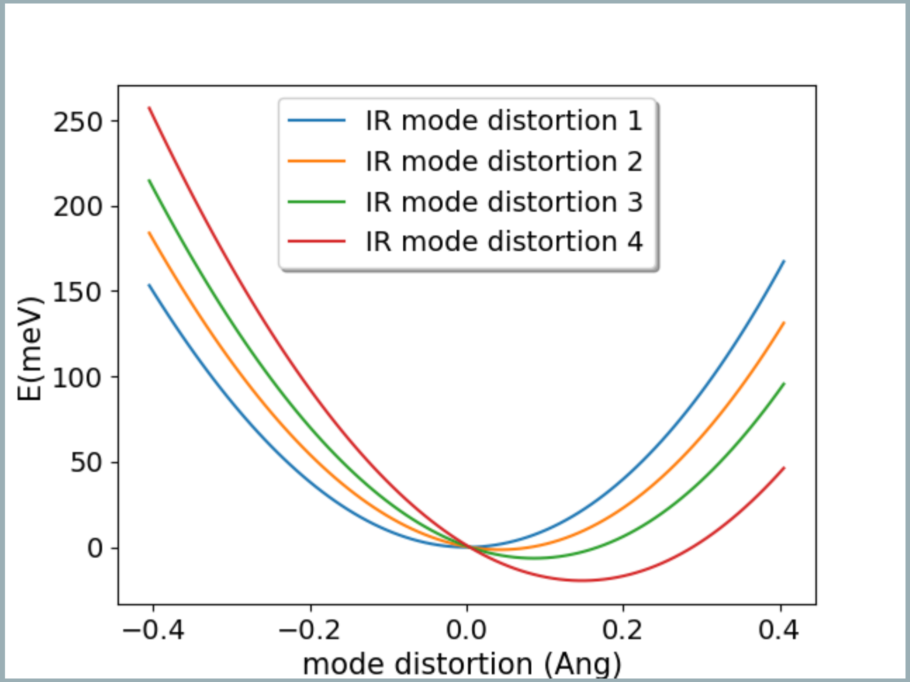
The two lowest Raman mods give the largest coupling with high frequency IR modes

	C_R	$d_I R$	d_R	γ_1
$A_g(1)$	-0.004	0.0072	0.000	0.0681
$A_g(2)$	0.003	0.0072	0.000	0.1246

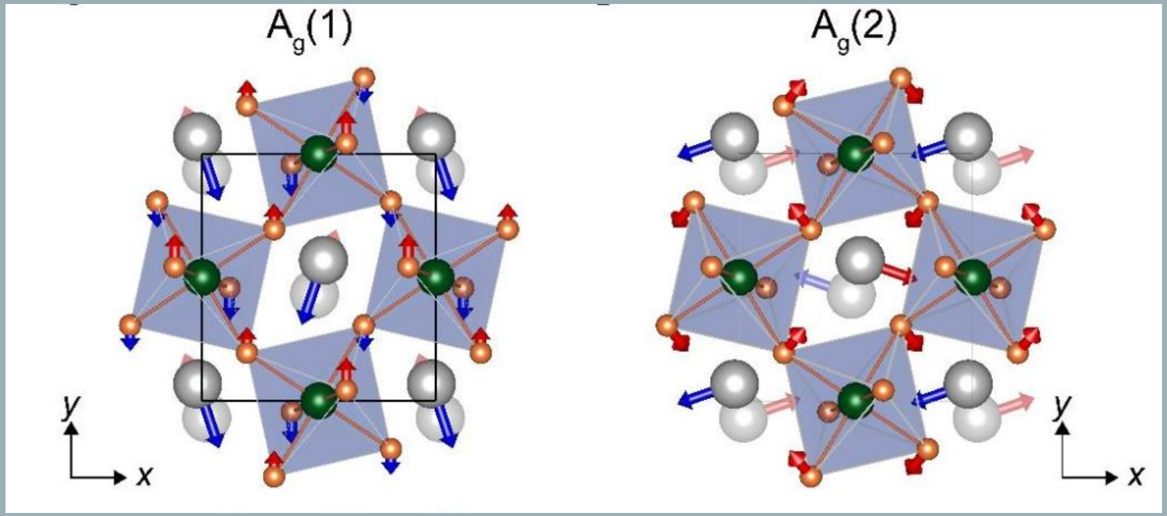
units meV/($\sqrt{amu}A$)^n

Phonon-phonon

❑ IR mode modifies potential energy surface for Ag mode



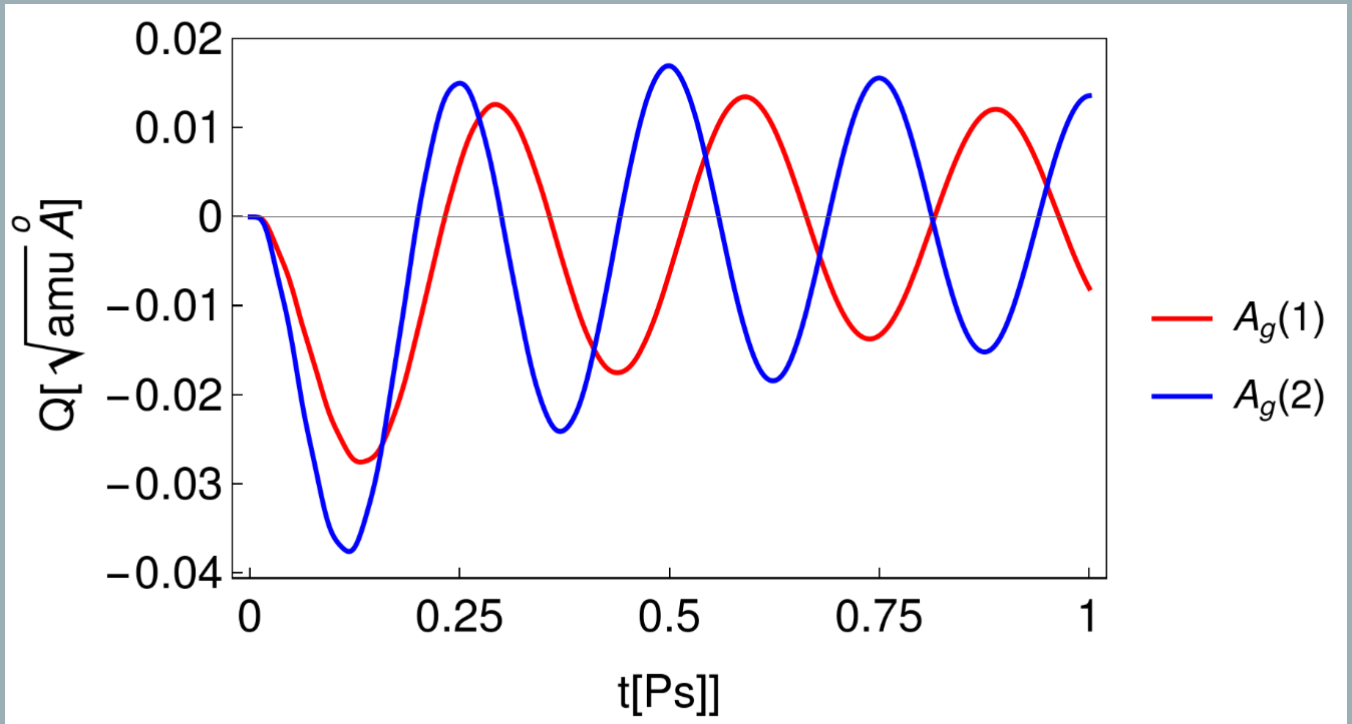
❑ This coupling can quasi statically induce some distortions
In the structure of A_g mode



Non linear phononics

- Dynamics of the modes equation of motion for the modes.

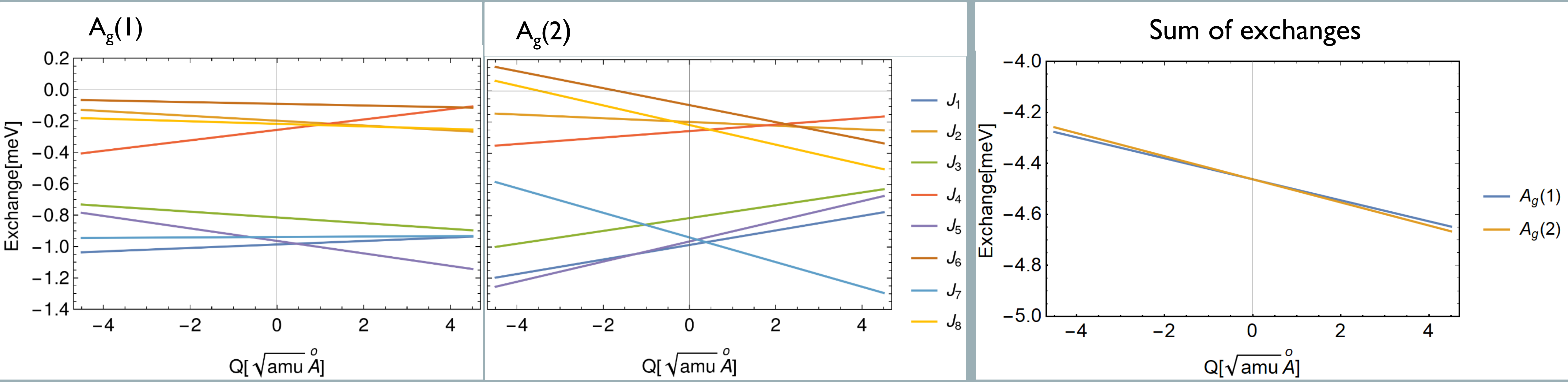
$$\ddot{Q} + \gamma \dot{Q} + \nabla_Q [V(Q) - F(t,Q) Q_{IR}] = 0$$



- Non linear Phonon couplings shifts the atoms according to Ag modes to a different position

- This can change the Properties of the material in time scales of several pico-seconds

Magnetic interactions in laser



- ❑ Low frequency mode distortions modify the interaction between the Dy atoms and Fe atom
- ❑ Ag modes change J(Dy-Fe) → induce magnetic phase transition (G1 → G4)

Conclusion

- Our findings shows the possibility of inducing magnetic phase transition with ferromagnetic order in very low time scale

Afanasiev et al., Nature Materials 20, 607 (2021)

Thanks you for your attention