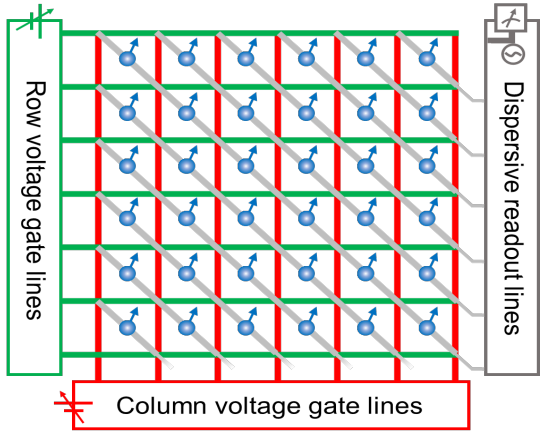

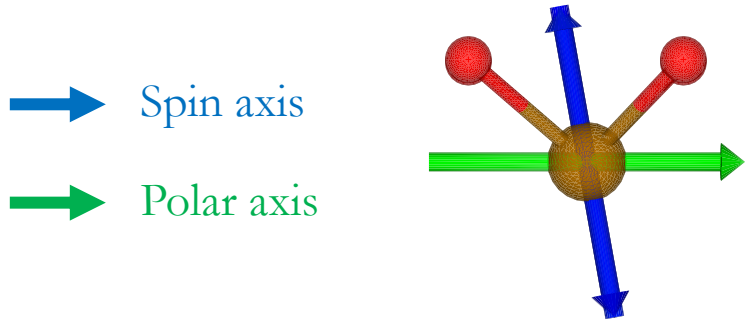

Electric field control of single spins in oxide ferroelectrics

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APS March Meeting 2021

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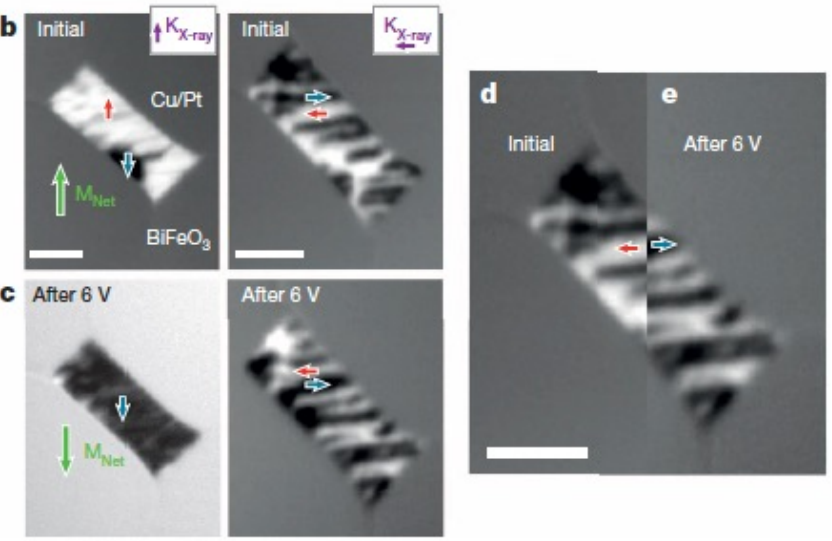
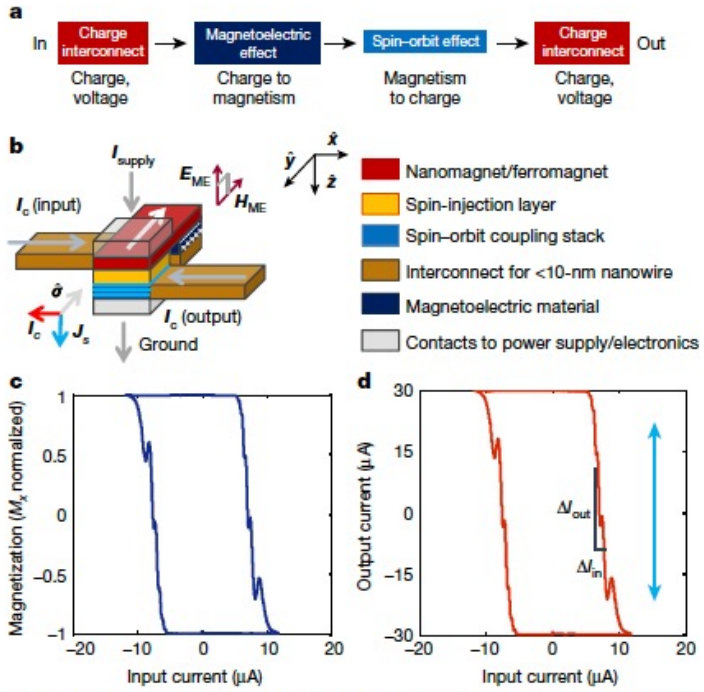
March 17, 2021

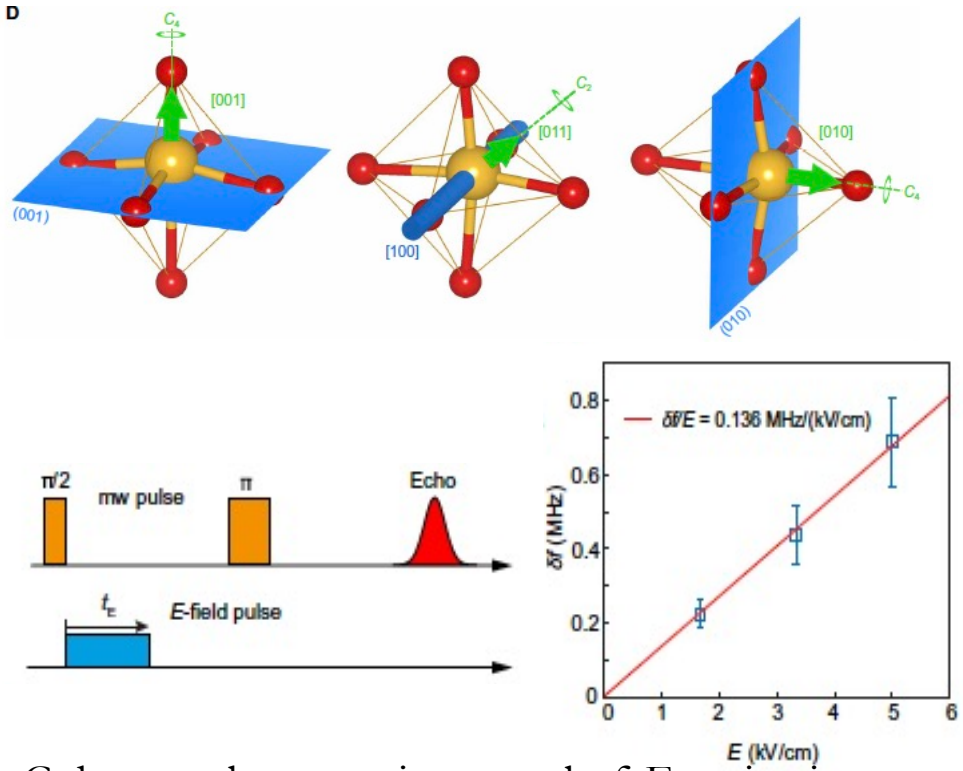
Electrostatic control of spins: past and present



Room temperature electrostatic switching of magnetisms in $BiFeO_3$ (2014)[1] [governed by DMI]



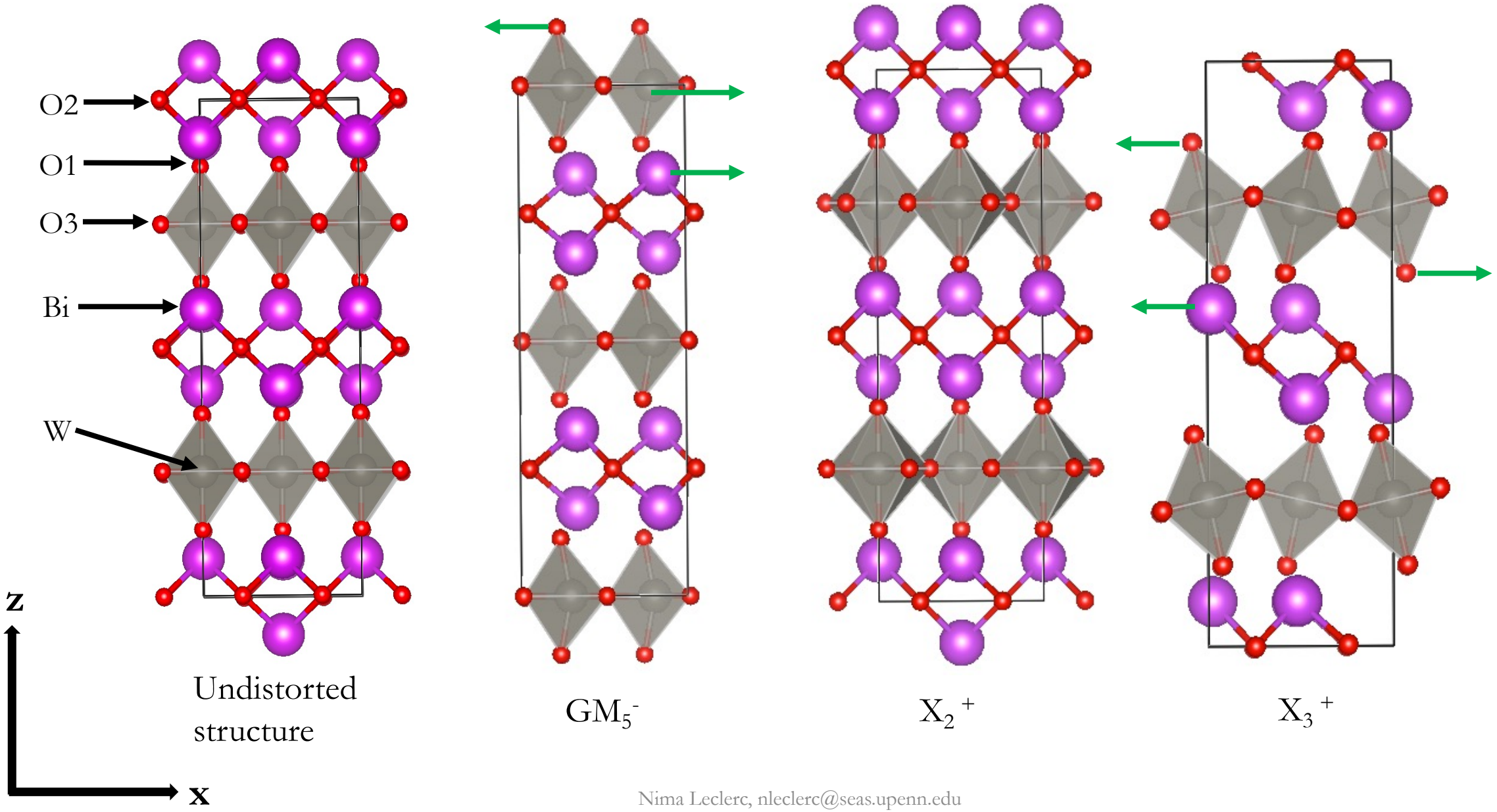
Electrostatic control of spins realized in non-volatile memory devices by Intel (2019)[2]



Coherent electrostatic control of Fe spins in $PbTiO_3$ [governed by SOC + CF] (2021)[3]

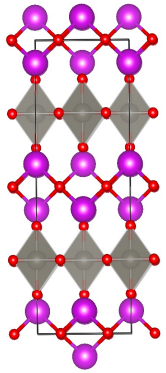
[1] *Nature* 18 Dec 2014: Vol. 516, pp. 370-373
[2] *Nature* 3 Jan 2019: Vol. 565, pp. 35-42
[3] *Science Advances* 03 Mar 2021: Vol. 7, no. 10, eabf8103

Bi_2WO_6 as a ferroelectric host



Our approach: predict potential spin switching pathways

Ferroelectric switching pathway predictions

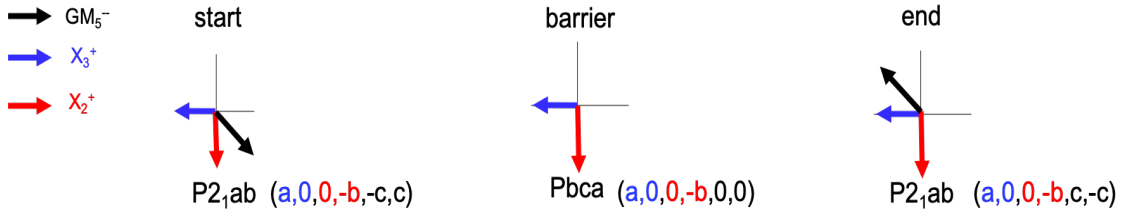


1. Solve for paraelectric structure

$$\frac{\delta E_{DFT}[n(\mathbf{r})]}{\delta n(\mathbf{r})}|_{n_0(\mathbf{r})} = 0$$

Generalized gradient approximation (GGA) within density functional theory (DFT)

2. Find lattice distortions in phase space



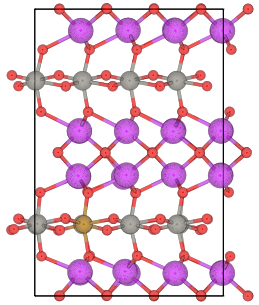
Map distortions to 2 domains corresponding to 2 energy minima: +/- **P** (start and end)

3. Use nudge elastic band to find intermediates

Predicts most energetically favorable combo of distortions ➔ correspond to metastable phases

Magnetic property predictions

4. Solve for relaxed Fe doped structures

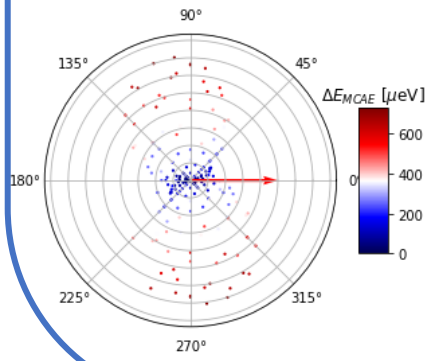


Substitute Fe ion in 2x2x1 supercell for each stable + metastable phase ➔ relax structure

5. Spin collinear + non-collinear calculations

Compute total energies of for collinear and non-collinear spin configurations. Use Hubbard-*U* correction and spin-orbit coupling

$$E_{DFT+U} = E_{DFT} + \frac{U}{2}\sum_s Tr[\rho^s - \rho^s\rho^s]$$

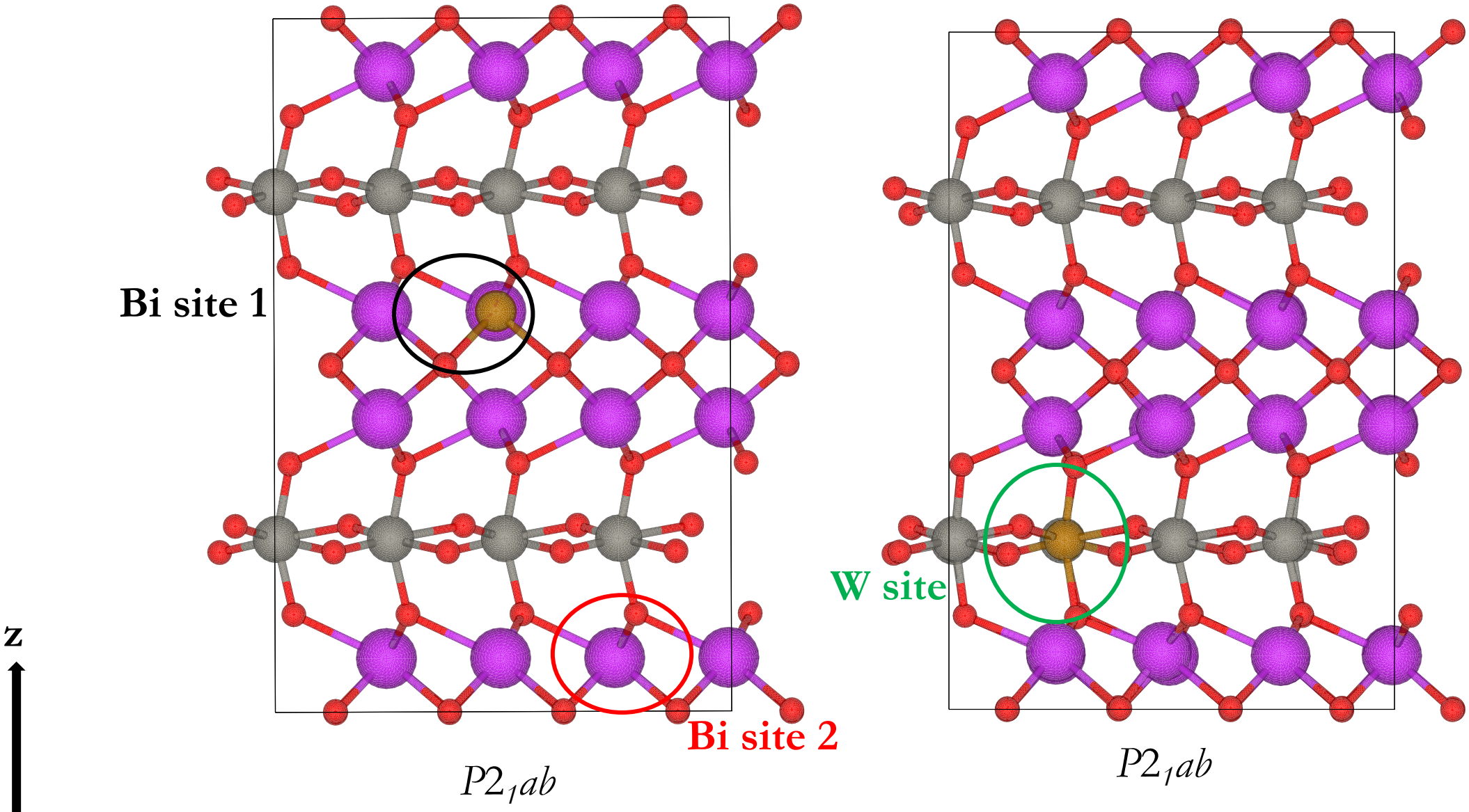


6. Obtain MCAE + easy axis

$$\Delta E_{MCAE}(\theta,\phi) = E(\theta,\phi) - E(\theta_{min},\phi_{min})$$

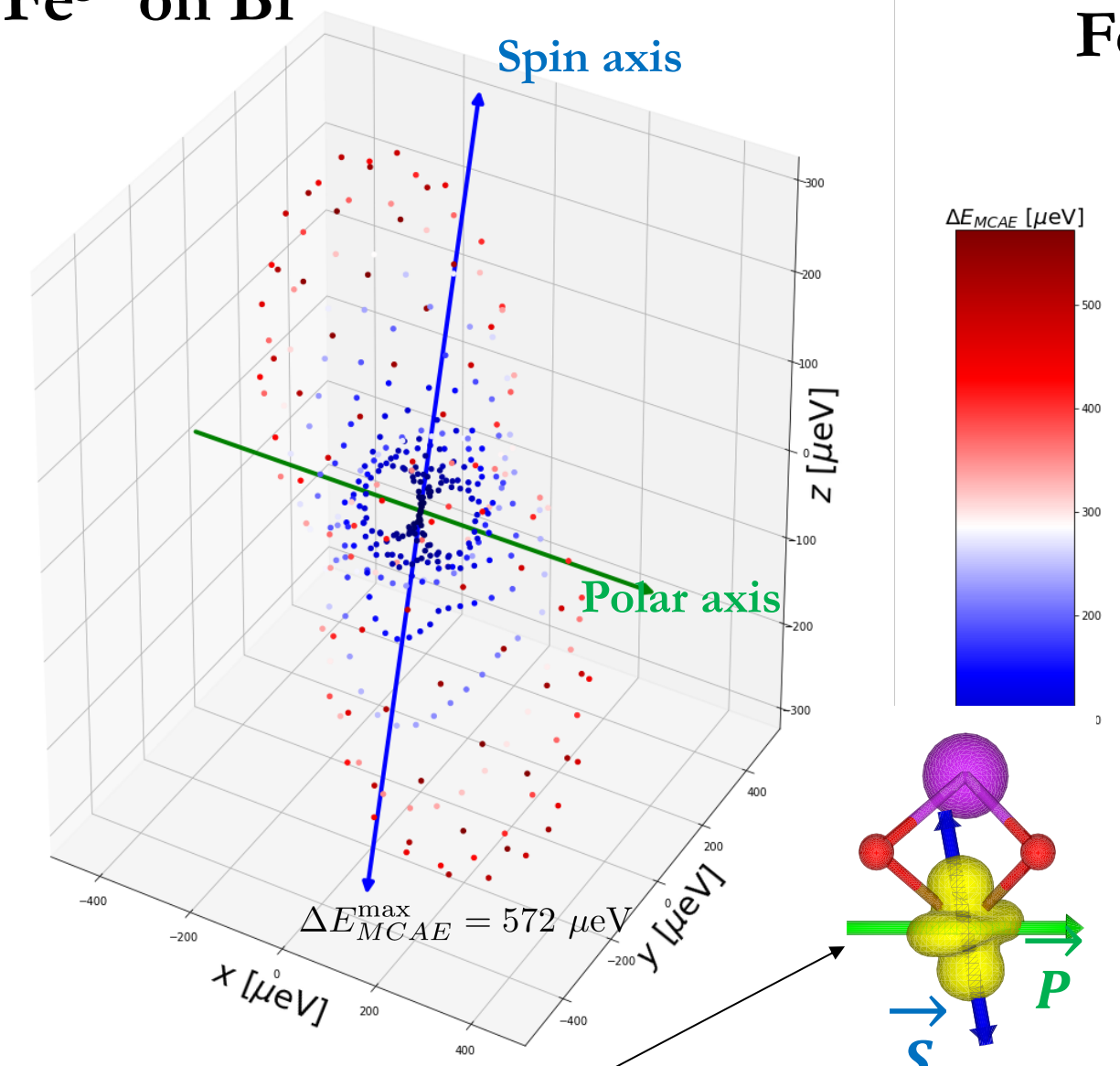
Calculate energy for multiple spin directions ➔ easy axis corresponds to lowest energy. Perform fit.

Fe^{3+} can sit on Bi or W sites in the Bi_2WO_6 host



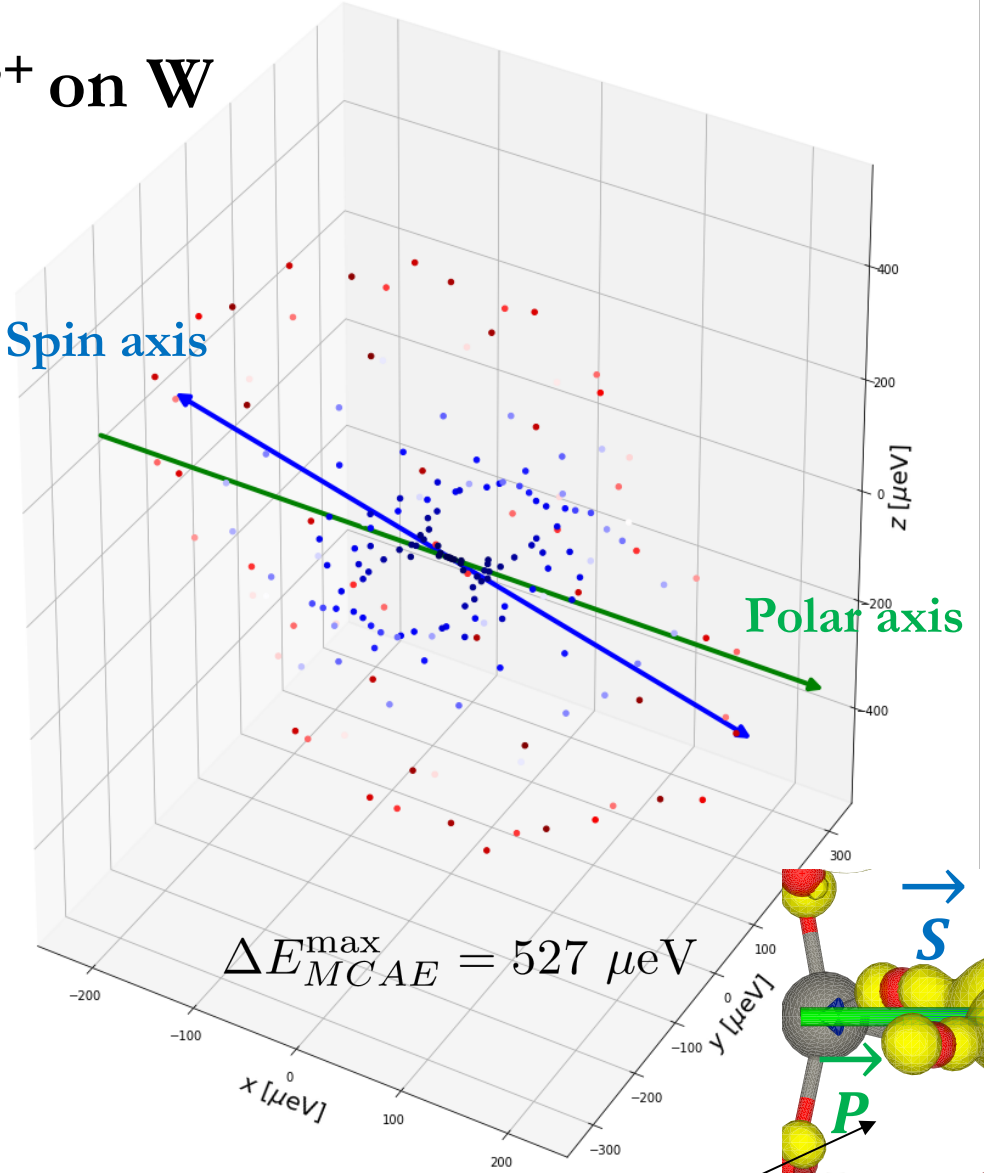
Magnetic anisotropy predictions for $P2_1ab$ [stable phase]

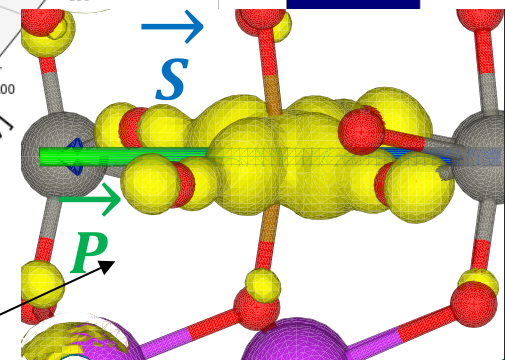
Fe^{3+} on Bi



$|d_{z^2}\rangle_{Fe}$

Fe^{3+} on W

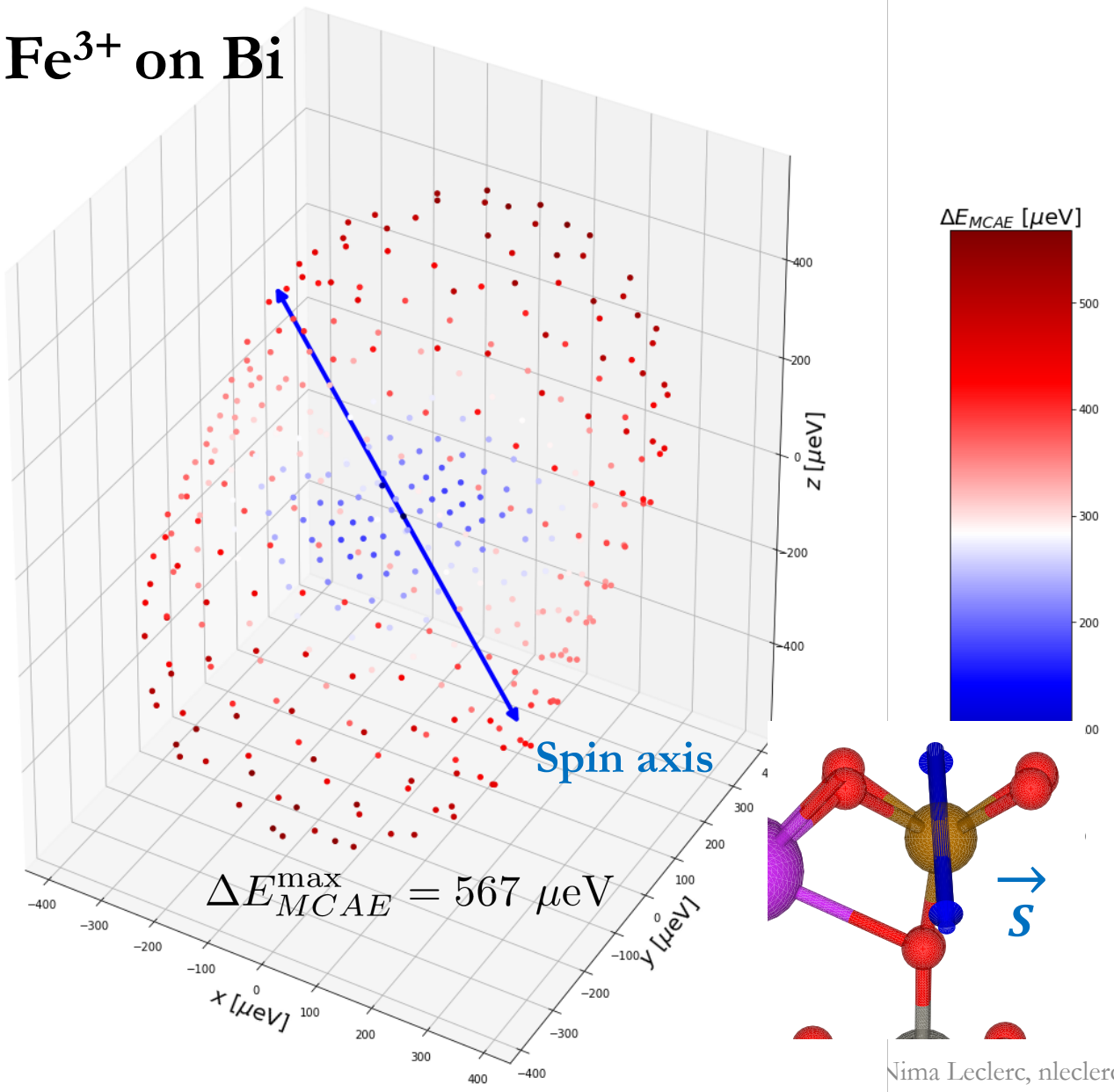




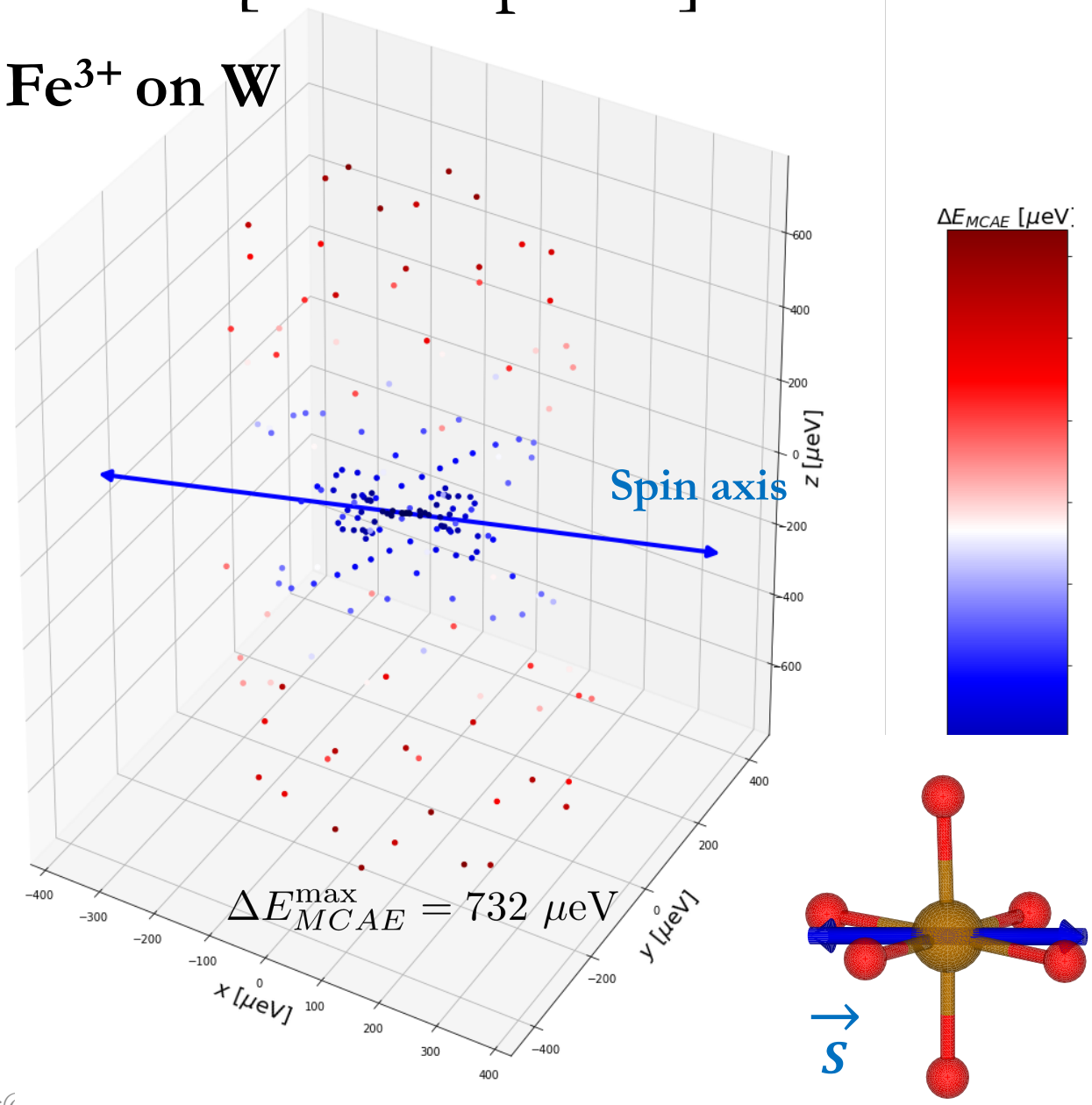
$|d_{x^2-y^2}\rangle_{Fe}$

Magnetic anisotropy predictions for *Pbca* [barrier phase]

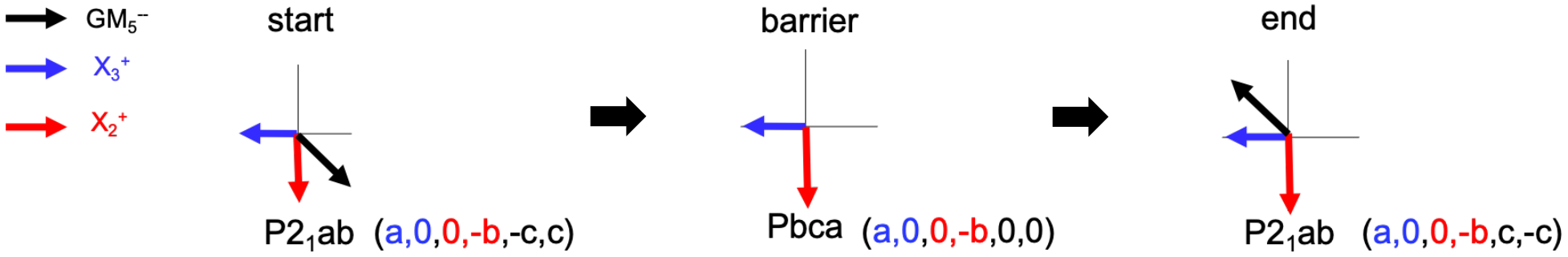
Fe^{3+} on Bi

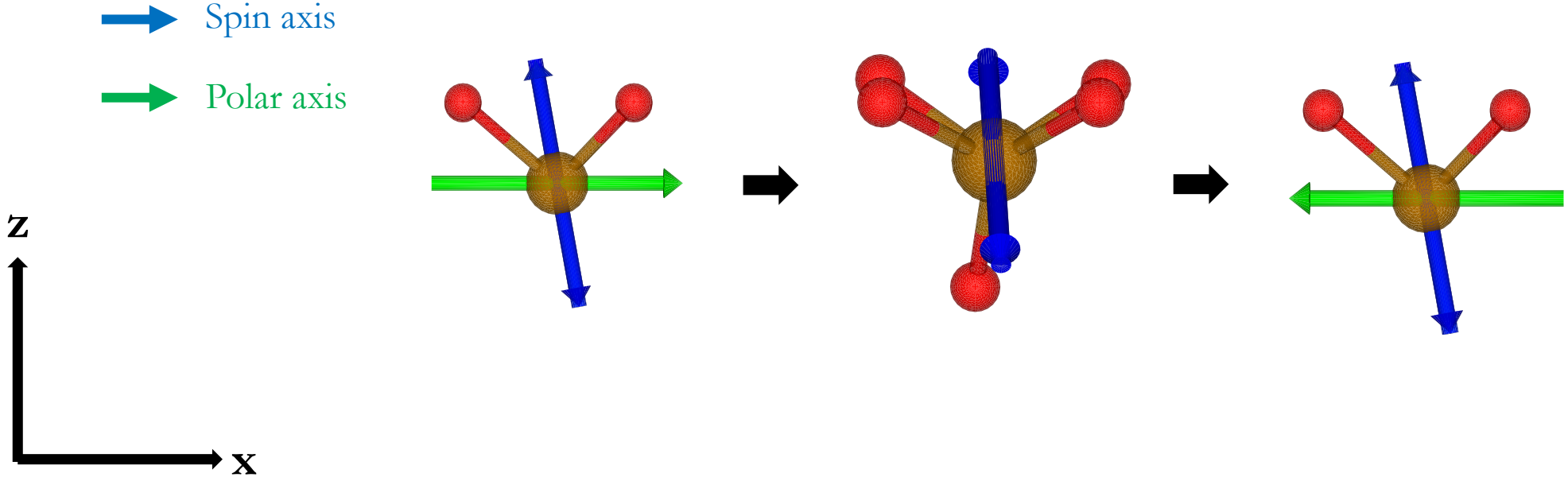


Fe^{3+} on W

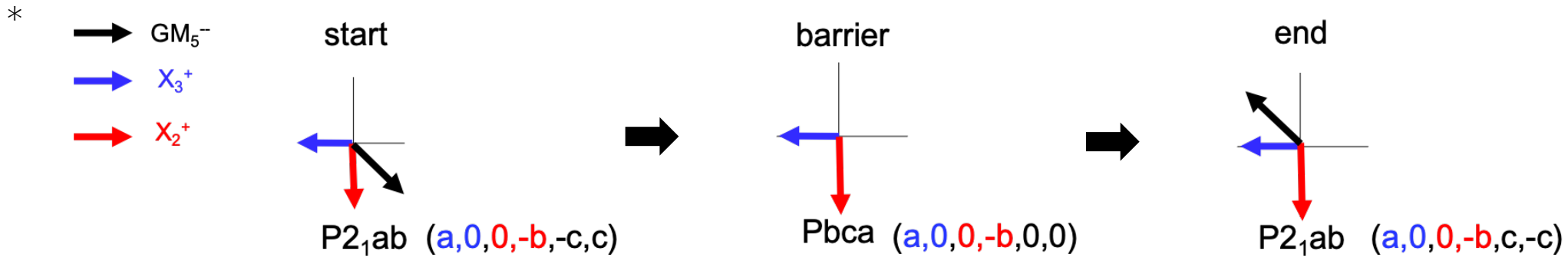


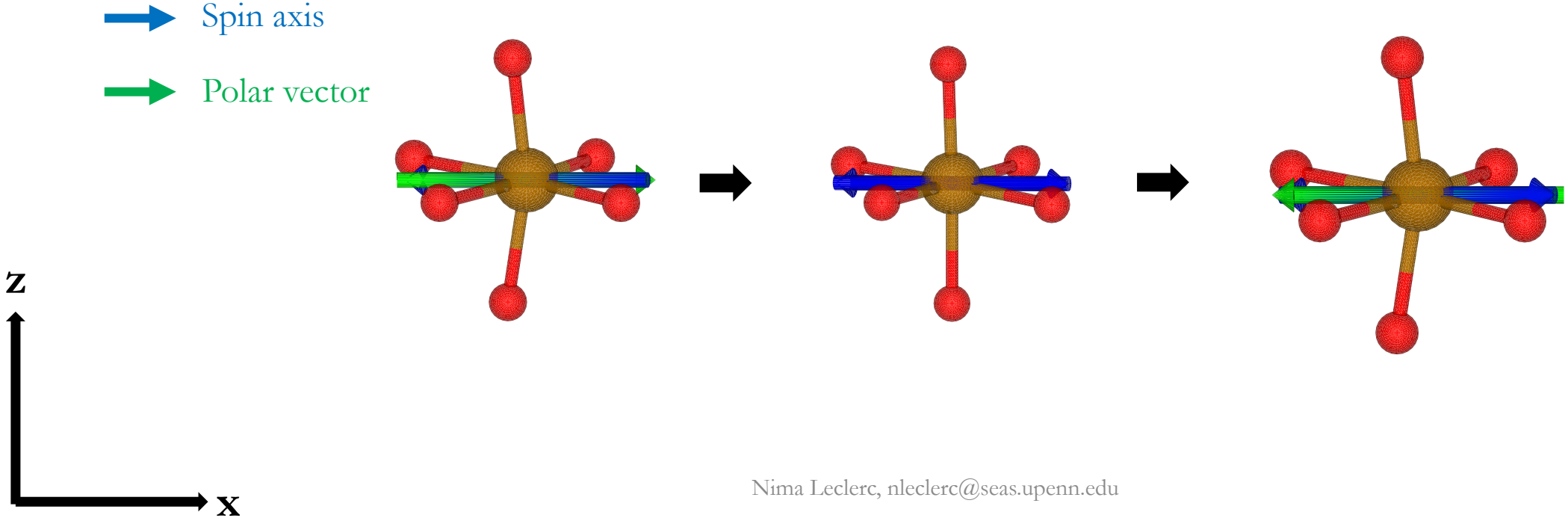
Polarization switching leads to spin switching: Fe^{3+} on Bi site





Polarization switching leads to spin switching: Fe^{3+} on W site





Conclusions and acknowledgments

- Spin-orbit coupling and distorted crystal field directly impacts the presence of a spin easy axis
- Ferroelectric Aurivillius phases have a rich compositional and low-symmetry phase space to explore new host materials
- Spin axis perpendicular to polarization for Fe on Bi site and parallel for Fe on W site
- Ongoing work: look at multi-step switching pathways, EPR measurements

Big thanks to Sinéad Griffin, Katherine Inzani, Elizabeth Nowadnick, and Nabaraj Pokhrel!

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*Supported by the Department of Energy Contract No. DE-AC02-05CH11231.