DiSPy Examples

Oxygen Diffusion on Graphene

Oxygen diffusion across a carbon ring on graphene can be used as a simple example to demonstrate the distortion symmetry method. Details regarding this example can be found in Ref. [4]. Linearly interpolating between the end states shown generates an initial path with a distortion symmetry group of m^*m2^*. Images for this path can be found in the "init_path" folder.

Running `DiSPy` with the sample input file will identify the distortion group, print out its irreducible representations, and perturb the images in the path according to distortion symmetry-adapted modes constructed using the Γ_2 irreducible representation. This can be found as no. 1259 in the listing by Stokes *et al.* [3], and produces a new initial path with a distortion group of m^*.

Ferroelectric Switching in $Ca_3Ti_2O_7$

Currently, there is a strong interest in ferroelectric materials that have a coupling between their polarization and another order parameter. Recently, a class of materials called hybrid improper ferroelectrics was predicted theoretically in n = 2 Ruddlesden-Popper (RP) materials, and shown experimentally in $Ca_3Ti_2O_7$ (CTO). This class of materials is characterized by their ferroelectricity being induced by octahedral rotations.

An initial ferroelectric switching pathway in $Ca_3Ti_2O_7$ can be made by linearly interpolating between initial and final stats of opposite polarization shown in Ref. [2]. This path has a distortion symmetry group of $Cmcm^*$, and can be found in the "init_path" folder.

Running `DiSPy` with the sample input file will identify the distortion group, print out its irreducible representations, and perturb the images in the path according to distortion symmetry-adapted modes constructed using the Y_{4+} irreducible representation. This can be found as no. 2857 in the listing by Stokes *et al.* [3], and produces a new initial path with a distortion group of $Pbcn^*$.

Ferroelectric Switching in $LiNbO_3$

$LiNbO_3$ is a commonly used ferroelectric material. The origin of its ferroelectricity can be traced to a polar mode associated with the displacement of the Li cations along the three-fold rhombohedral axis. Reversing the polarization of the structure then involves the motion of these cations along this axis [5].

Images for an initial ferroelectric switching pathway can be found in "init_path". These was constructed using a linear interpolation between the initial and final supercell images (2×2×2 rhombohedral unit cells) of opposite polarization which can be found in Ref.[5]s.

Running `DiSPy` with the sample input file will identify the distortion group, print out its irreducible representations, and perturb the images in the path according to distortion symmetry-adapted perturbations constructed using the F_{1+} irreducible representation. This can be found as no. 7611 in the listing by Stokes *et al.* [3]

The F_{1+} irreducible representation is three-dimensional, and is associated with the $k = (1/2, 1/2, 0)$ point. This means that coefficients for the order parameter vector need to be set in order to choose the appropriate isotropy subgroup, and that there will be a loss in translational symmetry after perturbation. This loss is characterized by all of the k-vectors in the star of the wave-vector $\{k = (1/2, 1/2, 0), (0, 1/2, 1/2), (1/2, 0, 1/2)\}$, and is appropriately accommodated by the 2×2×2 supercell.

Since we would like to break the most amount symmetry in this case, the isotropy subgroup associated with the kernel of the irreducible representation is desired. This corresponds to $P\bar{1}^*$, and can be obtained by choosing three distinct entries for the order parameter vector: $\eta = (0.8, 1.0, 1.4)$. This information can be found using the `ISOSUBGROUP` listing by Stokes *et al.* [3]

Rigid Sliding in $MoTe_2$

The rigid sliding between layers in 2D materials is of interest to characterize atomic contributions to nanoscale friction in the material. This example concerns the rigid sliding path for $MoTe_2$ shown in Ref. [1].

An initial path can be made by linearly interpolating between the initial and final states shown in Ref. [1]. This path has a distortion symmetry group of $Cmcm$, which does not contain distortion reversal symmetry (starred elements). Nonetheless, the same procedure may be applied.

Running `DiSPy` with the sample input file will identify the distortion group, print out its irreducible representations, and perturb the images in the path according to distortion symmetry-adapted perturbations constructed using the Γ_{3+} irreducible representation.

This can be found as no. 2836 in the listing by Stokes *et al.* [3], and produces a new initial path with a distortion symmetry group of $C2/m$.

References

[1] A. Cammarata and T. Polcar. Overcoming nanoscale friction barriers in transition metal dichalcogenides. *Physical Review B*, 96(8):085406, Aug. 2017.

[2] E. a. Nowadnick and C. J. Fennie. Domains and ferroelectric switching pathways in $Ca_3Ti_2O_7$ from first principles. *Physical Review B*, 94(10):104105, Sept. 2016.

[3] H. T. Stokes, B. J. Campbell, and R. Cordes. Tabulation of irreducible representations of the crystallographic space groups and their superspace extensions. *Acta Crystallographica Section A Foundations of Crystallography*, 69(4):388–395, July 2013.

[4] B. K. VanLeeuwen and V. Gopalan. The antisymmetry of distortions. *Nature Communications*, 6:8818, 2015.

[5] M. Ye and D. Vanderbilt. Ferroelectricity in corundum derivatives. *Physical Review B*, 93(13):134303, Apr. 2016.