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DFPT vs TDEP

Boris Dorado

CEA, France

- Phonons in a nutshell: compute **derivatives of the total energy**. Can be **analytical** or **numerical**.
- Analytical: solve the **Sternheimer equation** (aka the « derivative » of the Schrödinger equation).
→ Density Functional Perturbation Theory, DFPT ([Baroni *et al.*, Rev. Mod. Phys. 73, 515 \(2001\)](#))
- Numerical: perform **finite differences**.
→ Finite displacements.
- DFPT:
 - Pros:
 - ❖ Analytical → **most accurate**.
 - ❖ Calculations on primitive unit cells → **fastest**.
 - ❖ Phonons calculated analytically on any \mathbf{q} point → **not size dependent**.
 - ❖ No size dependency → defects, alloys, etc.
 - Cons:
 - ❖ The maths are ugly → **hinders implementation** (electron correlations, spin-orbit coupling, etc.)
 - ❖ No temperature effects → **extrapolation** to finite T with **(quasi)harmonic approximation**.
 - ❖ Not very useful for phases that are **dynamically unstable at OK**.

➤ Finite displacements:

- Pros:
 - ❖ **Conceptually simple**: possible with any *ab initio* code.
 - ❖ Finite **temperature effects** (molecular dynamics)
- Cons:
 - ❖ Numerical → **less accurate** than DFPT.
 - ❖ Primitive cell → Γ point only. Other \mathbf{q} points require (very) **large supercells**.
 - ❖ Supercell is be mapped back onto the primitive cell → **perfect crystals** or **substitutional defects**.
 - ❖ *Ab Initio* Molecular Dynamics (AIMD) can take months → **computationally demanding**.