

# Must-read references:

PHYSICAL REVIEW B **93**, 195137 (2016)

## **Second-principles method for materials simulations including electron and lattice degrees of freedom**

Pablo García-Fernández,<sup>1</sup> Jacek C. Wojdel,<sup>2</sup> Jorge Íñiguez,<sup>2,3</sup> and Javier Junquera<sup>1</sup>

J. Phys.: Condens. Matter **25** (2013) 305401 (25pp)

doi:10.1088/0953-8984/25/30/305401

## **First-principles model potentials for lattice-dynamical studies: general methodology and example of application to ferroic perovskite oxides**

Jacek C Wojdel<sup>1</sup>, Patrick Hermet<sup>2,3</sup>, Mathias P Ljungberg<sup>1</sup>, Philippe Ghosez<sup>2</sup> and Jorge Íñiguez<sup>1</sup>

PHYSICAL REVIEW B **95**, 094115 (2017)

## **Efficient systematic scheme to construct second-principles lattice dynamical models**

Carlos Escorihuela-Sayalero,<sup>1</sup> Jacek C. Wojdel,<sup>2</sup> and Jorge Íñiguez<sup>1,2</sup>

# **Very important note!**

**SCALE-UP models may be analogous to pseudo-potentials in a DFT code...**

**BUT**

**They are not nearly as robust or simple!**

**SO**

**You have to know what you are doing!!**

# Starting point

- This is a project at its initial stages, and we don't really know how it will (we want it to) look like 10 years from now.
- What we do know is that the approach/methods are complex and not mature enough yet.
- So, for now, our approach is a bit conservative (slow, but safe), as regards users, distribution, etc.
- Which should be compatible with doing many things!, but not just with \*everybody in the world\* doing many things.
- From users, we ask: a lot of feedback (& a bit of patience), help us improve/complete the approach/code

# License for SCALE-UP and the MODELMAKERS

! SCALE-UP, version 0.0.0, July 2017

! SCALE-UP core team:

! - P. Garcia-Fernandez and J. Junquera (U. Cantabria)

! - J. Iniguez (Luxembourg Inst. Science and Technology)

! Contributors to this version:

! - C. Escorihuela-Sayalero (Luxembourg Inst. of Science and Technology)

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Registered SCALE-UP users can modify the code according to their needs. Users must communicate significant changes of the code to the SCALE-UP core team. The core team will have the right to include such modifications in future versions of SCALE-UP, acknowledging the corresponding users as contributors.

# Philosophy

- New users & distribution → Jorge
- (Major) Developments → Jorge
- Bug reports → Pablo
- Models → Pablo
- Web page → [www.secondprinciples.unican.es](http://www.secondprinciples.unican.es)