Material science problems on IBiSCo

Valentina Barreca
Cesma (Centro Servizi Metrologici e Tecnologici Avanzati)
Dipartimento di Fisica Ettore Pancini, Unina

18-19/04/2024

Why the need of using IBiSCo?

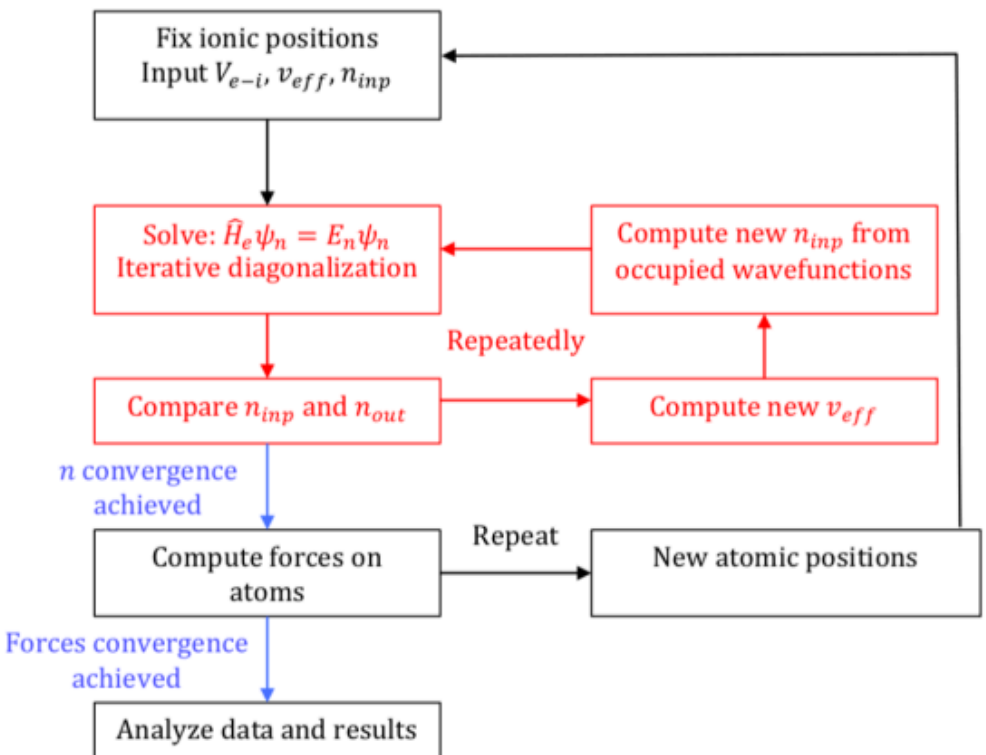
Simulations of materials in their ground states using the Quantum Espresso package (QE): an integrated suite of open-source computer codes for electronic structure calculations based on density functional theory

- Large number of parameters
- Use of large plane waves basis sets
- Autoconsistency and numerous iterations
- Generation of large temporary folders

Resolution of the Kohn-Sham self-consistent equations

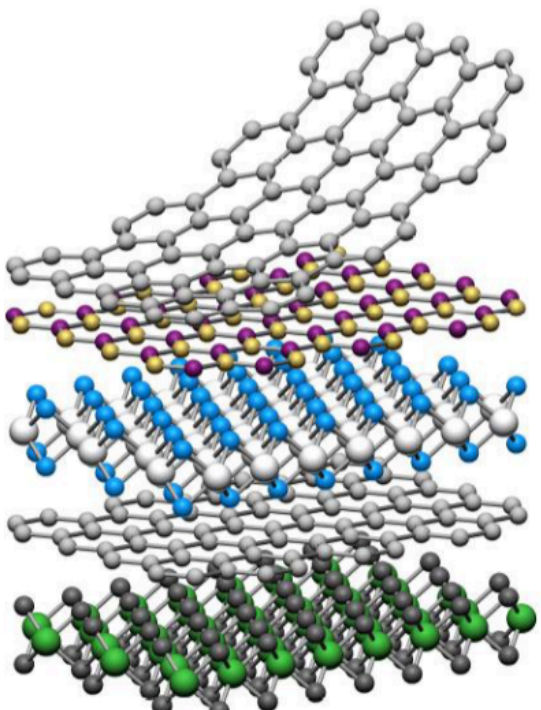
$$\left[-\frac{1}{2}\nabla^2{}_r + v_{\text{eff}}\ (r) - \varepsilon_j\right]\psi_j = 0$$

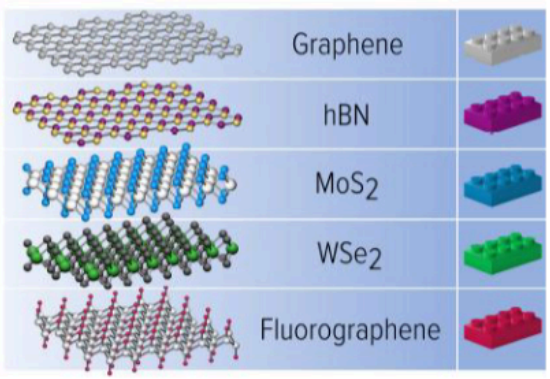
$$v_{\text{eff}} = v^{\text{ext}}\ (r) + \frac{\delta E^{\text{xc}}}{\delta n} + \int d^3r' \frac{n(r)}{|r - r'|}$$

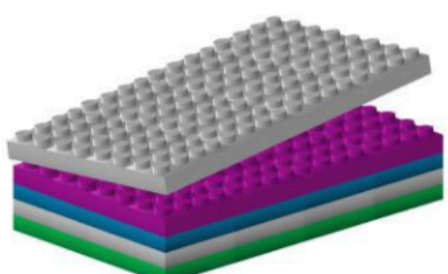


Two-dimensional materials simulations

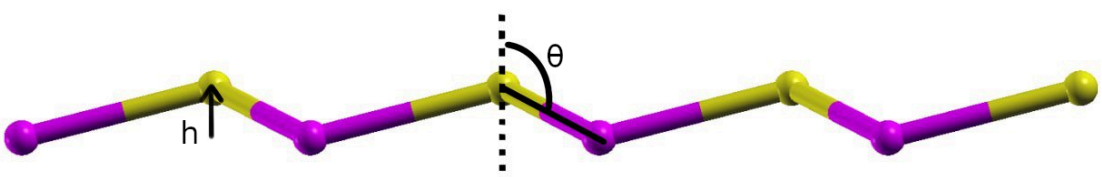
Two-dimensional materials stacked on top of each other as lego blocks in order to tune their properties

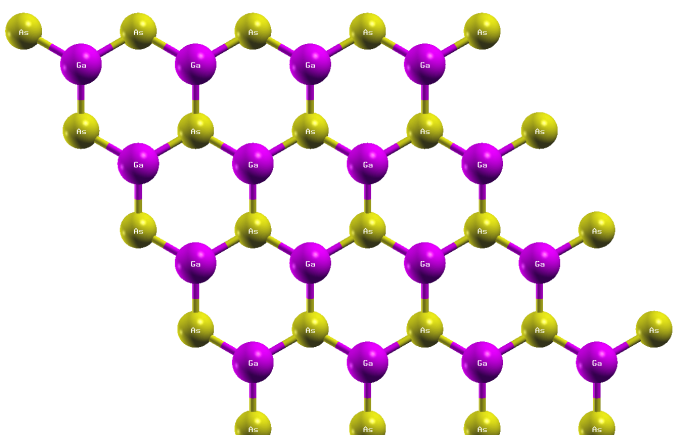


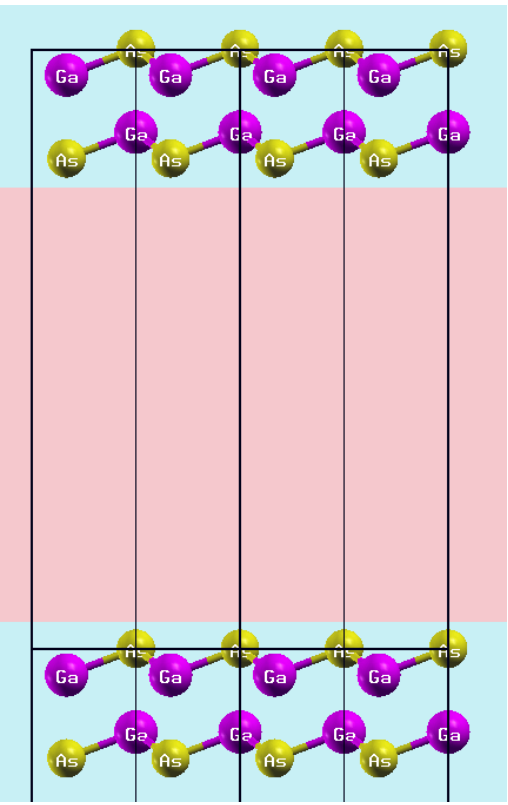




Using of QE on IBiSco to simulate some two-dimensional buckled binary compounds and to study their properties, such as band structures and density of states.

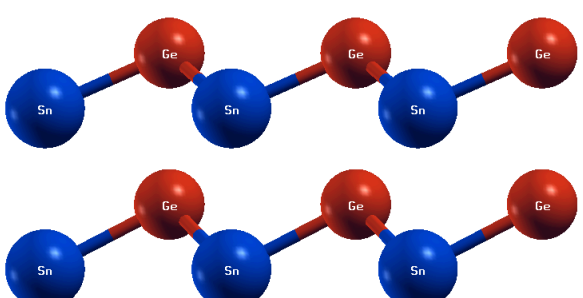


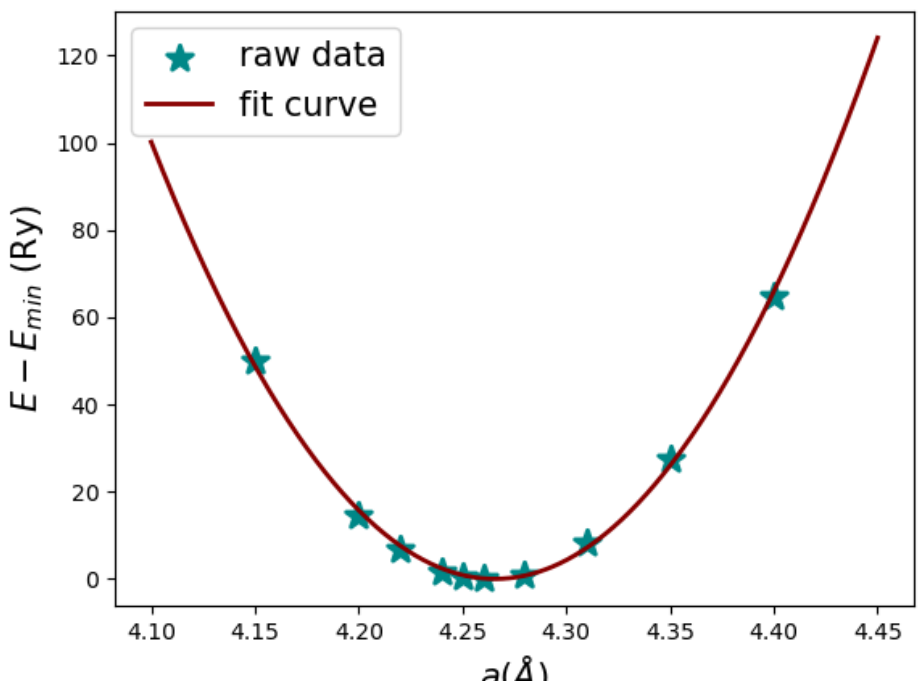




- Structures made of more layers
- Empty space in the out-of-plane direction
- Sample of the Brilluoin zone with a finite number of k-points

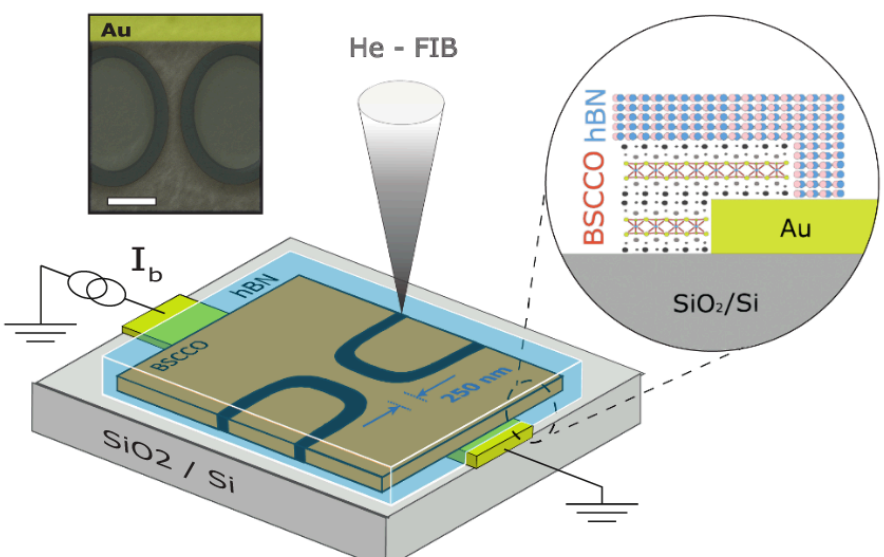
Application of an in-plane strain for a GeSn bilayer: the optimized lattice parameter is 4.26 Å, against 4.31 Å of the monolayer



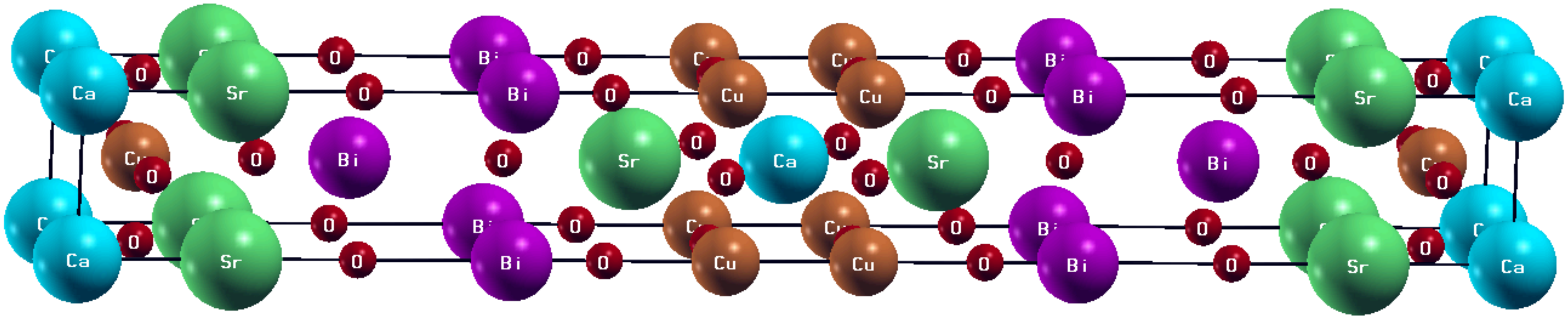


Cuprate simulations

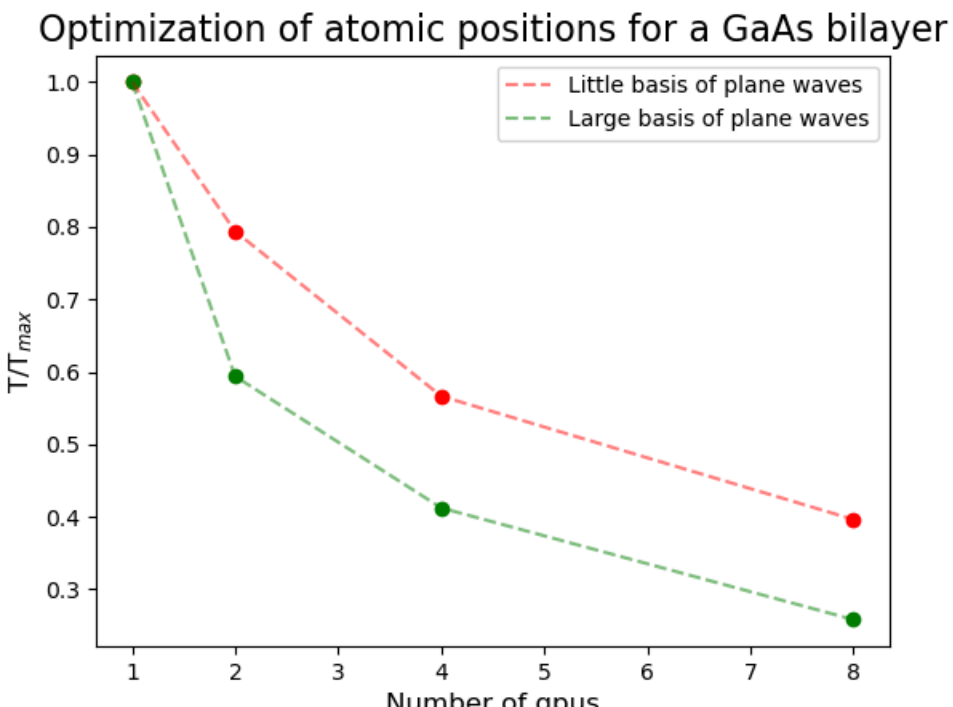
$Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO) is a layered material, useful in the fabrication of single-photons detectors



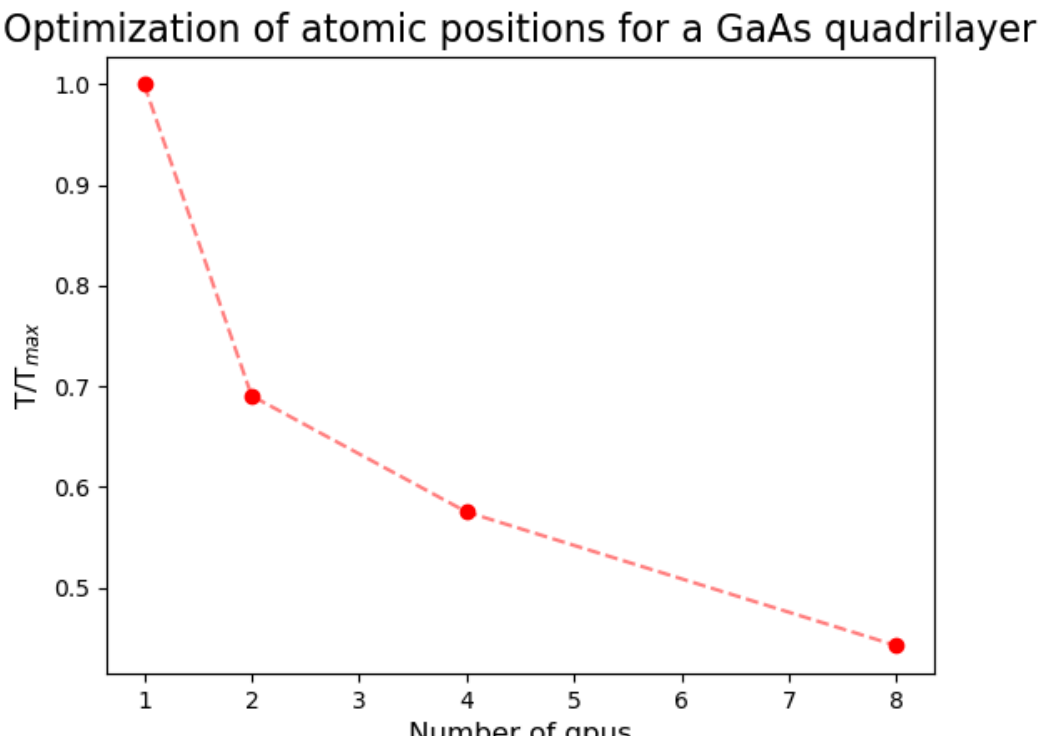
- Unit cell containing 15 atoms
- Unit cell that can be described with a simple (30 atoms/cell, 260 electrons) or body-centered (15 atoms/cell, 130 electrons) tetragonal lattice



Benchmarking



- 4 atoms/cell, 36 electrons
- 34 k-points
- Different plane wave basis set in the two cases



Improved complexity:

- 8 atoms/cell, 72 electrons
- 34 k-points
- Higher income from 1 to 2 gpus

Thanks for the attention!