News from Padova

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BSE without GW

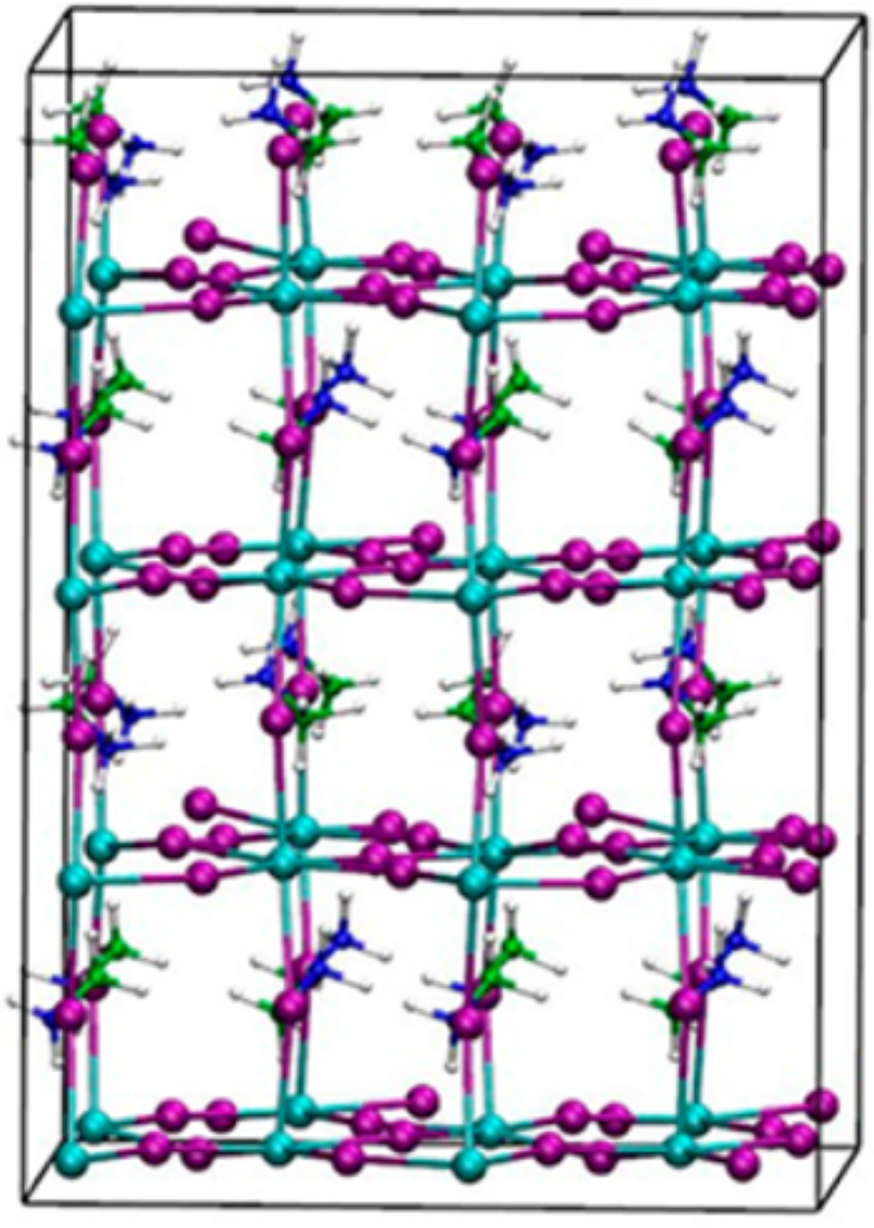
- **BSE code without empty states (with optional Wannier for N^3 scaling) has been modified for calculating W_c using linear response using DFPT.**
- **GW no longer required for the W_c**
- **for the quasi particle energy level GW can be replaced by Koopman compliant DFT, maybe hybrids(?)**
- **only NC and Gamma only**
- **inserted in GWW/bse to be committed**
- **work done with J. Elliot (CNR-IOM) and N. Colonna, N.Marzari (EPFL)**
- **one paper to be submitted soon**

The simple code

- **new code as pw.x post-processing for calculating dielectric properties (dielectric functions) with RPA and BSE**
- **RPA with intra and interband terms (also for metals)**
- **based on Shirley's basis:one common basis for the periodic part of the KS wave-functions of all the k-points**
- **for BSE it uses an optimally reduced basis for product functions**
- **SOC is supported**
- **NC only**
- **explicit sums over empty states**
- **W_c at the moment only from GWL code (can be ported to other GW codes)**
- **now part of the GWL package to be inserted in git (?)**
- **in collaboration with G. Prandini , N. Marzari (EPFL)**
- **in used for automatised materials search**
- **paper in preparation**

Example:

MAPbI3: 384 atoms
SOC calculation
2x2x2 k-points grid
64 cores
12h



P.Umari, E. Mosconi, F. De Angelis, J. Phys. Chem. Lett. 9, 620 (2018).

What about?

A new QE development school for beginners?
(with new documentation)

An active real workshop for QE developers?