Latest news from Padova

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1. A new BSE code

- no empty states
- interfaced with GWL code for W operator
- based on Wannier's functions
- accuracy/computational cost controlled with one single parameter (overlap of Wannier's)
- only Gamma point sampling / real wave functions
- truncated Coulomb interaction and treatment of extended systems
- now in private GWL project on qe-forge
- finishing now last tests / preparing first papers

- what to do now? Probably in GWW QE-package!
- the same scheme could be easily extended to TD-DFT
- interface with other GW codes?

1. A new BSE code

How does it work? e.g. exchange part of direct term (TD-HF)

$$|\psi_v\rangle$$

$$|w_v\rangle = \sum_{v'} U_{vv'} |\psi_{v'}\rangle$$

$$\langle vc| K^{d,x} |v'c'\rangle = -\int d\mathbf{r}d\mathbf{r}'\psi_c(\mathbf{r})\psi_c(\mathbf{r})v(\mathbf{r},\mathbf{r}')\psi_{v'}(\mathbf{r})\psi_{v'}(\mathbf{r})$$

$$A = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \cdots \\ \phi_{N_v} \end{pmatrix}$$

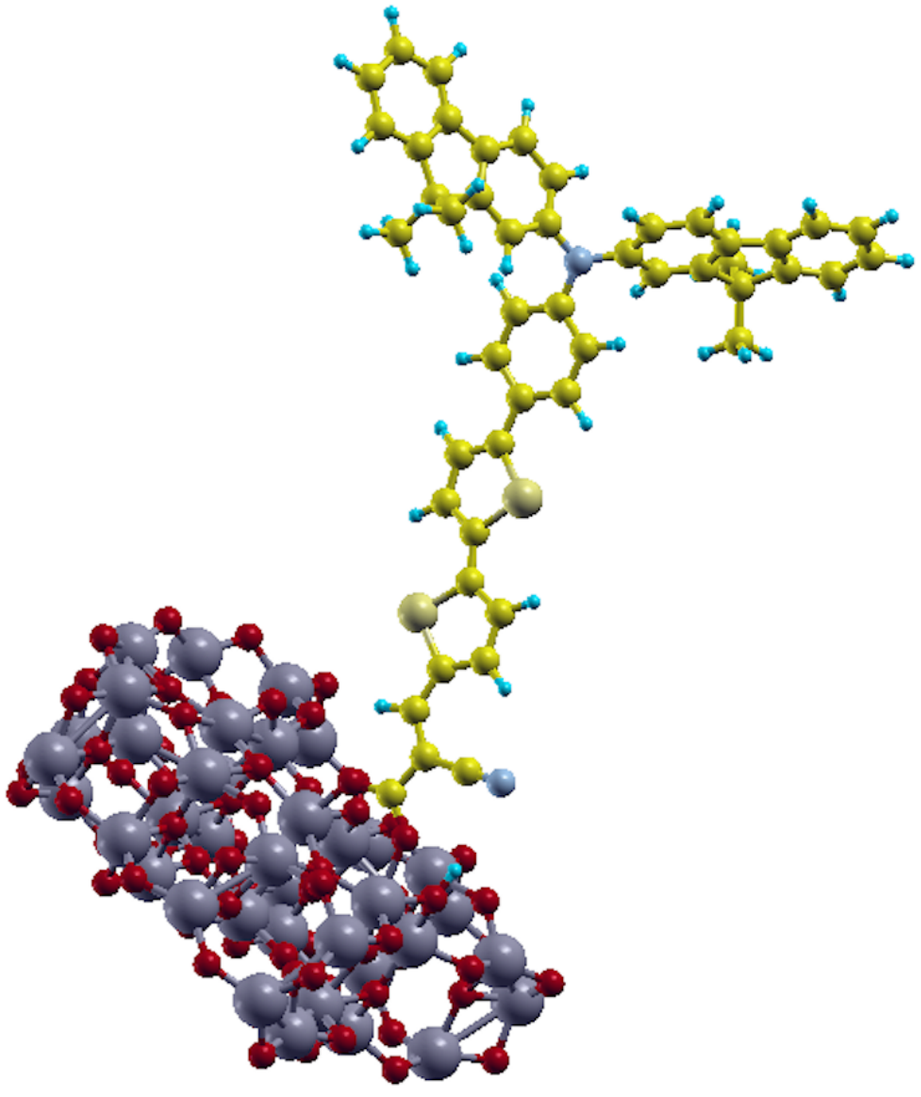
$$A' = \begin{pmatrix} \sum_{v'} U_{1v'}\phi_{v'} \\ \sum_{v'} U_{2v'}\phi_{v'} \\ \cdots \\ \sum_{v'} U_{N_v v'}\phi_{vi} \end{pmatrix} = \begin{pmatrix} \phi'_1 \\ \phi'_2 \\ \\ \phi'_{Nv} \end{pmatrix}$$

$$\langle vc| K^{d,x} |v'c'\rangle = -\int d\mathbf{r}d\mathbf{r}'\psi_c(\mathbf{r})\psi_c(\mathbf{r})v(\mathbf{r},\mathbf{r}')w_{v'}(\mathbf{r})w_{v'}(\mathbf{r})$$

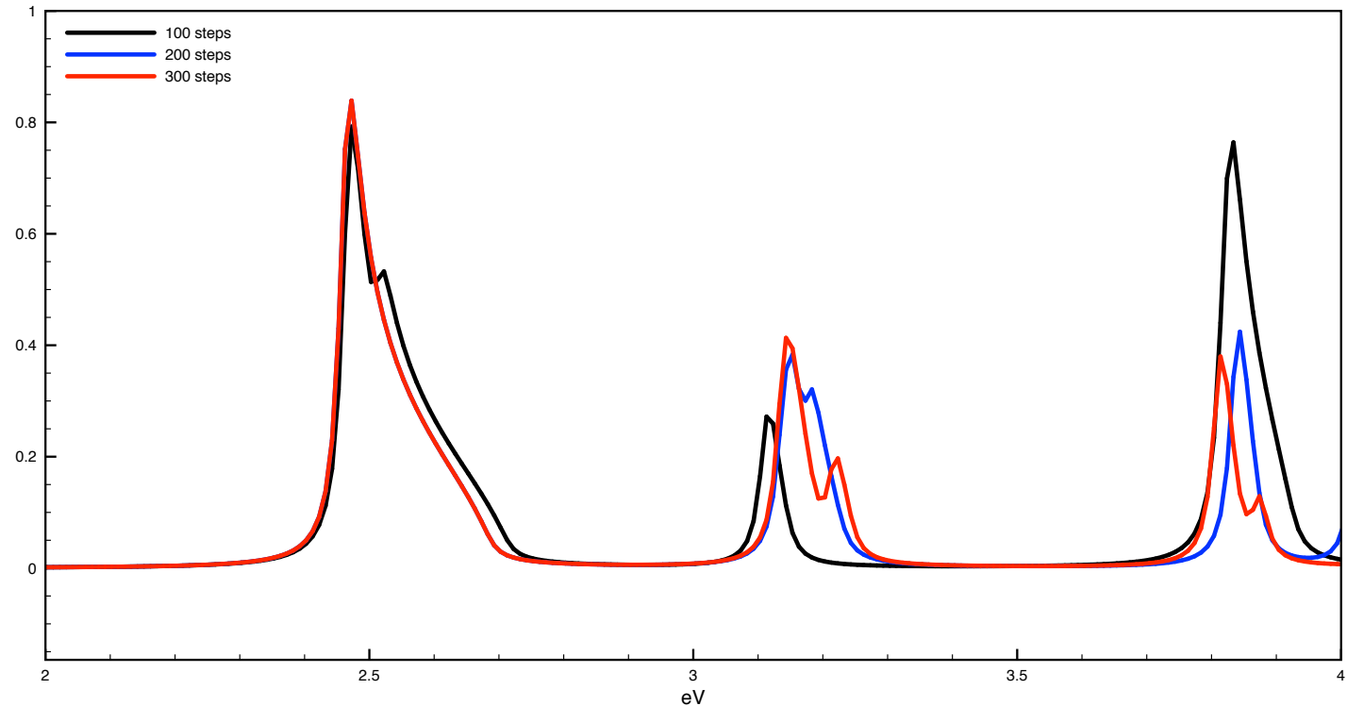
$$K^{d,x}|A'\rangle = \begin{pmatrix} \int d\mathbf{r}' P_c(\mathbf{r},\mathbf{r}') \sum^*_{v'} \phi'_{v'}(\mathbf{r}') (vw_1 w_{v'})(\mathbf{r}') \\ \\ d\mathbf{r}' P_c(\mathbf{r},\mathbf{r}') \sum^*_{v'} \phi'_{v'}(\mathbf{r}') (vw_{N_v} w_{v'})(\mathbf{r}') \end{pmatrix}$$

$$(vw_v w_{v'})(\mathbf{r}) = \int d\mathbf{r}' v(\mathbf{r},\mathbf{r}') w_v(\mathbf{r}') w_{v'}(\mathbf{r}')$$

1. A new BSE code



JK2@TiO_2



2. Another one…

- almost for witz…
- based on Shirley's basis and on product basis
- explicit sums over empty states
- k-points
- US pseudos
- SOC
- at a good development point
- will be used by master students

- is anyone interested in the thing?

3. TURBO EXX

- For gapped systems Coulomb operator entering Fock operator can be made periodic
- only certain G are required
- they can be obtained folding the FFT N^3 times, with N replica in the 3 cart. directions
- no Wannier's functions required, can be applied to delocalized states
- (was) implemented in a private version of pw.x even with task-groups over bands

- what to do now?

3. TURBO EXX

TABLE I. Total energy, Fock contribution to the total energy, HOMO and LUMO energies calculated at the HF level with different energy cutoff and with different schemes for benzene. The total computational time required by the evaluation of the Fock operator and relative speed-ups are also shown. The used energy cutoff (in Ry) is shown besides the scheme label.

	Total energy (Ry)	Fock energy (Ry)	Fock-term HOMO (eV)	Fock-term time (s)	Fock-term speed-up
STANDARD/40 Ry	−73.088	−22.987	−9.18	0.4550	1.0
FAST/40 Ry	−73.088	−22.987	−9.19	0.1548	3.4
TURBO/40 Ry	−73.089	−22.990	−9.18	0.0449	9.9
STANDARD/80 Ry	−73.425	−23.016	−9.21	1.3707	1.0
FAST/80 Ry	−73.425	−23.016	−9.21	0.5509	2.5
TURBO/80 Ry	−73.424	−23.017	−9.21	0.1719	8.0

TABLE II. Results of PBE0 self-consistent calculations for the H_2TPP molecule through STANDARD, FAST, and TURBO.

	Total energy (Ry)	Fock energy (Ry)	HOMO (eV)	LUMO (eV)	Total time (min)	Speed-up
STANDARD	−615.485	−44.212	−5.28	−2.29	1564	1.0
FAST	−615.485	−44.212	−5.28	−2.29	704	2.2
TURBO	−615.488	−44.215	−5.26	−2.32	286	5.5

TABLE IV. Results of PBE0 self-consistent calculations for a 512 atoms model of bulk Si with a random displacement of each atom from its equilibrium geometry. The global calculation time and the average computer time of the Fock-term subroutine are reported.

	Total energy (Ry)	Fock energy (Ry)	Mean force per atom (Ry/a.u.)	Mean error on force (Ry/a.u.)	HOMO (eV)	LUMO (eV)	Fock-term time (s)	Fock-term speed-up	Total time (min)	Global speed-up
STANDARD	−4031.54	−271.25	0.0297	0.000	5.42	7.11	0.64	1	5201	1
FAST	−4031.54	271.25	0.0297	0.000	5.42	7.11	0.40	1.6	3258	1.6
TURBO	−4030.86	270.72	0.0299	0.005	5.40	7.11	0.13	5.1	1710	3.0