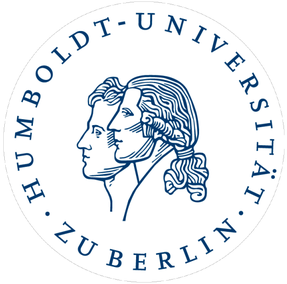
Hybrid functionals in exciting

HoW exciting! 2023

Cecilia Vona, HU Berlin

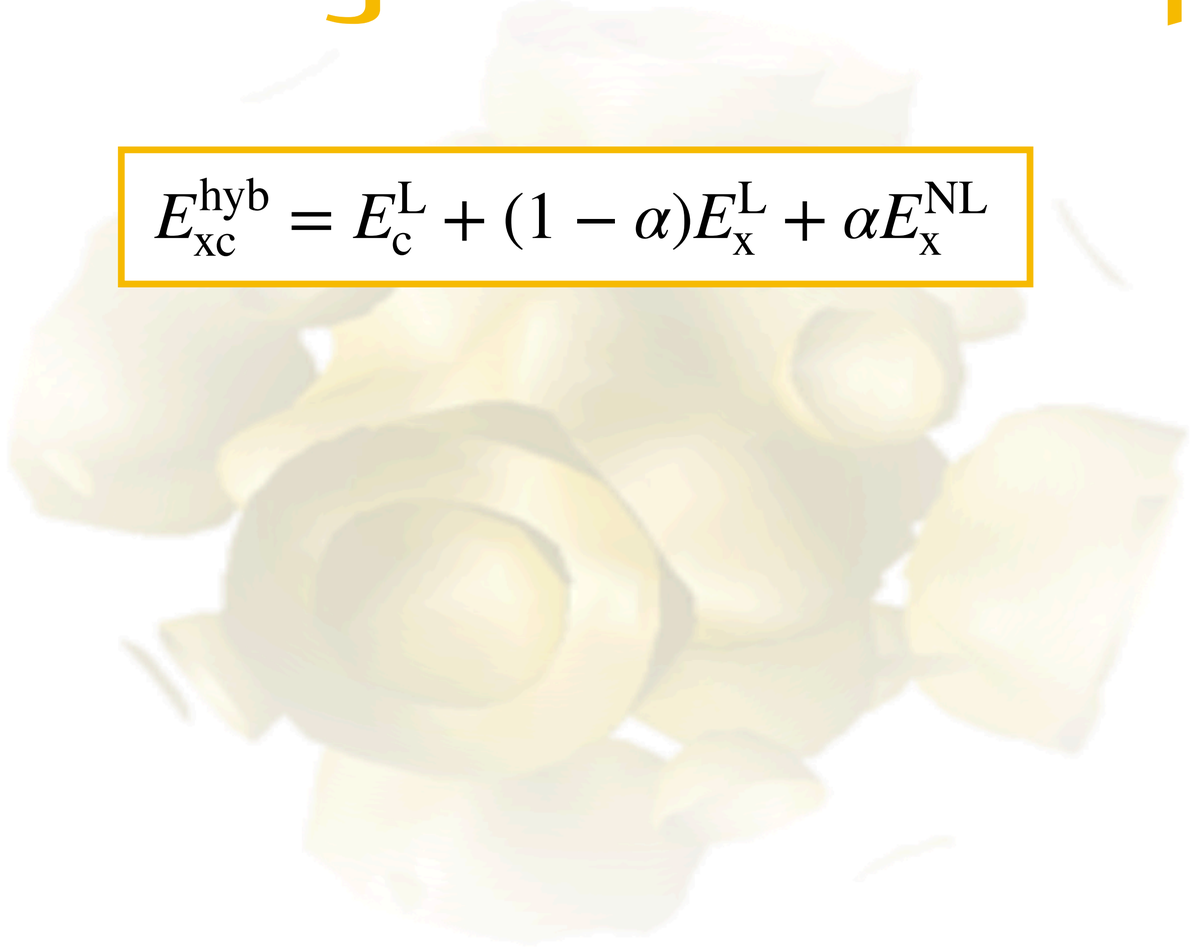


Time line

- Introduction
- Implementation in **exciting**
- Running basic calculations
- Advanced parameters
- Parallelization
- Additional features

Hybrid exchange-correlation functionals

$$E_{\mathrm{xc}}^{\mathrm{hyb}} = E_{\mathrm{c}}^{\mathrm{L}} + (1-\alpha)E_{\mathrm{x}}^{\mathrm{L}} + \alpha E_{\mathrm{x}}^{\mathrm{NL}}$$



Hybrid exchange-correlation functionals

$$E_{xc}^{hyb} = E_c^L + (1-\alpha)E_x^L + \alpha E_x^{NL}$$

PBE0

$$E_{xc}^{PBE0} = E_{xc}^{PBE} + \alpha\left[E_x^{NL} - E_x^{PBE}\right] \quad \text{with} \quad \alpha = 0.25$$

Adamo *et al., J. Chem. Phys*. **110**, 6158 (1999); Ernzerhof *et al., J. Chem. Phys.* **110**, 5029 (1999)

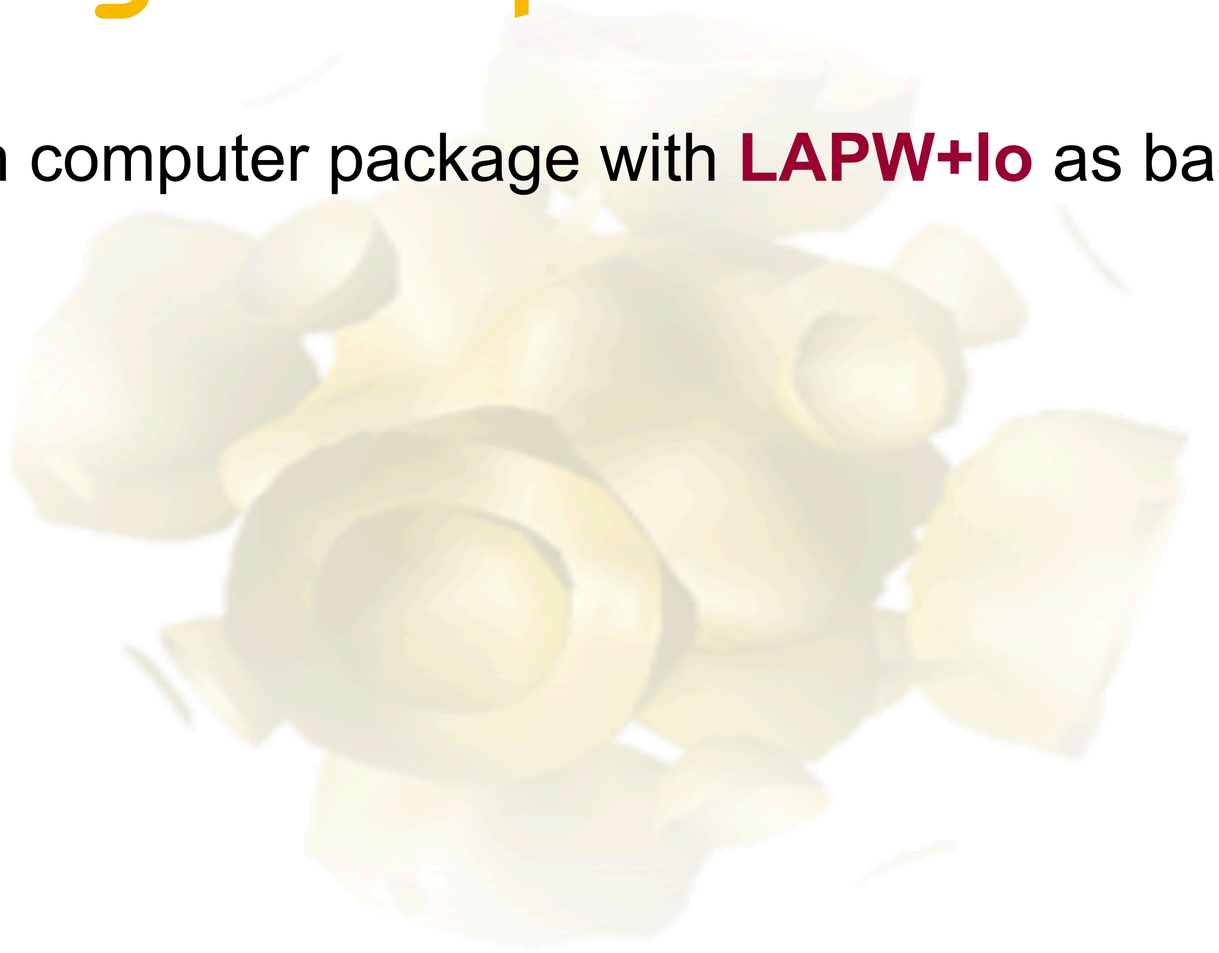
HSE06

$$E_{xc}^{HSE06} = E_{xc}^{PBE} + \alpha\left[E_x^{NL,SR}(\omega) - E_x^{PBE,SR}(\omega)\right] \quad \text{with} \quad \alpha = 0.25, \ \omega = 0.11\ a_0^{-1}$$

Heyd *et al.*, *J. Chem. Phys.* 118, 8207 (2003) + Erratum *J. Chem. Phys.* 124, 219906 (2006);
Krukau *et al. J. Chem. Phys.* 125, 224106 (2006)

exciting basis functions

All-electron computer package with **LAPW+lo** as basis functions



Gulans *et al.*, *J. Phys.: Condens. Matter* **26**, 363202 (2014)

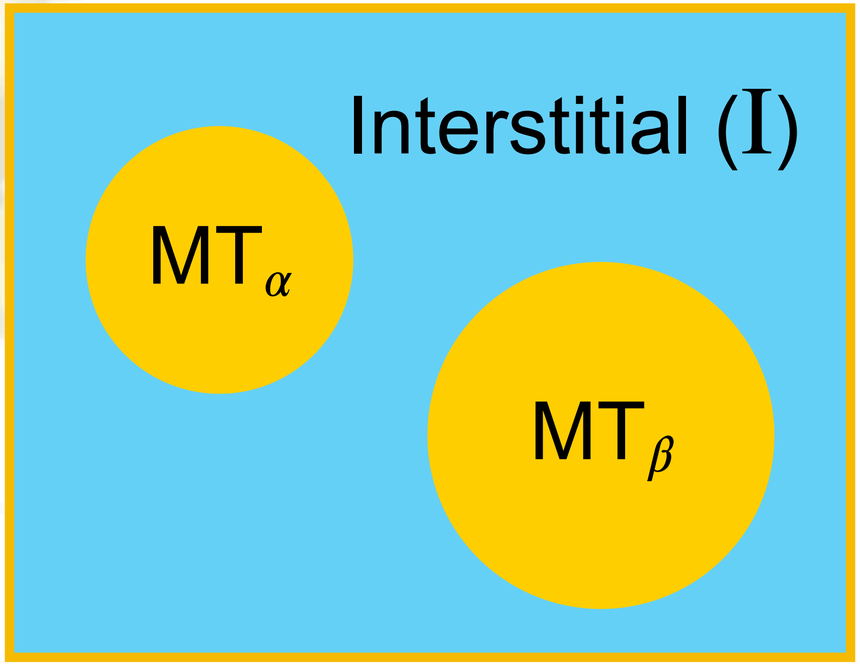
exciting basis functions

All-electron computer package with **LAPW+lo** as basis functions

KS wavefuctions: $$\varphi_{n\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} c^{\mathbf{k}}_{n\mathbf{G}} \phi_{\mathbf{G}+\mathbf{k}}(\mathbf{r})$$

APW basis functions:

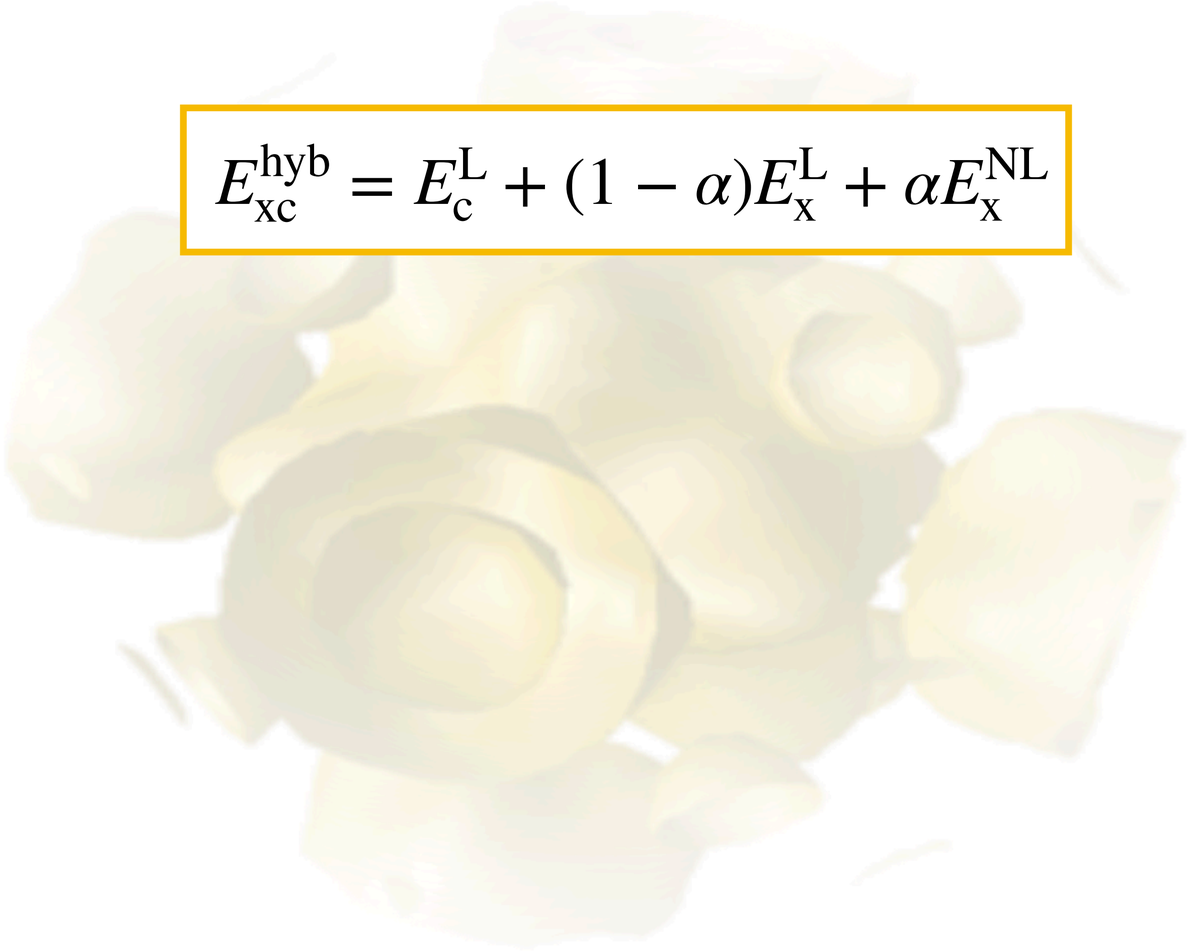
$$\phi_{\mathbf{G}+\mathbf{k}}(\mathbf{r}) = \begin{cases} \sum_{lm} A^{\mathbf{G}+\mathbf{k}}_{lm\alpha} u_{l\alpha}(r_\alpha) Y_{lm}(\hat{\mathbf{r}}_\alpha) & r_\alpha \leq R_{\mathrm{MT}} \\ \frac{1}{\sqrt{\Omega}} e^{i(\mathbf{G}+\mathbf{k})\cdot\mathbf{r}} & \mathbf{r} \in \mathrm{I} \end{cases}$$



Gulans *et al.*, *J. Phys.: Condens. Matter* **26**, 363202 (2014)

Hybrid functionals in **exciting**

$$E_{\mathrm{xc}}^{\mathrm{hyb}} = E_{\mathrm{c}}^{\mathrm{L}} + (1-\alpha)E_{\mathrm{x}}^{\mathrm{L}} + \alpha E_{\mathrm{x}}^{\mathrm{NL}}$$



Betzinger *et al., Phys. Rev. B* 81, 195117 (2010); H. Jiang *et al.,Comp. Phys. Comm.* 184, 348–366 (2013)

Hybrid functionals in **exciting**

$$E_{\mathrm{xc}}^{\mathrm{hyb}} = E_{\mathrm{c}}^{\mathrm{L}} + (1-\alpha)E_{\mathrm{x}}^{\mathrm{L}} + \alpha E_{\mathrm{x}}^{\mathrm{NL}}$$

Generalized Kohn-Sham equation:

$$h(\mathbf{r})\varphi_{n\mathbf{k}}(\mathbf{r}) + \alpha \int V_{\mathrm{x}}^{\mathrm{NL}}(\mathbf{r},\mathbf{r}')\varphi_{n\mathbf{r}'}d\mathbf{r} = \varepsilon_{n\mathbf{k}}\varphi_{n\mathbf{k}}(\mathbf{r})$$

L one-particle Hamiltonian

$$h(\mathbf{r}) = -\frac{1}{2}\nabla^2 + V_{\mathrm{ext}}(\mathbf{r}) + V_{\mathrm{H}} + V_{\mathrm{xc}}^{L}(\mathbf{r})$$

NL exact exchange potential

$$V_{\mathrm{x}}^{\mathrm{NL}}(\mathbf{r},\mathbf{r}') = -\sum_{n}^{\mathrm{occ.}}\sum_{\mathbf{k}}^{\mathrm{BZ}}\frac{\varphi_{n\mathbf{k}}(\mathbf{r})\varphi_{n\mathbf{k}}^{*}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

Betzinger *et al., Phys. Rev. B* 81, 195117 (2010); H. Jiang *et al.,Comp. Phys. Comm.* 184, 348–366 (2013)

Hybrid functionals in **exciting**

NL matrix elements

$$V^{\mathrm{NL}}_{\mathrm{x},nn'}(\mathbf{k}) = -\sum_{n''}^{\mathrm{occ}} \sum_{\mathbf{k}'}^{\mathrm{BZ}} \iint \frac{\varphi^*_{n\mathbf{k}}(\mathbf{r})\varphi_{n''\mathbf{k}'}(\mathbf{r})\varphi^*_{n''\mathbf{k}'}(\mathbf{r}')\varphi_{n'\mathbf{k}}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}d\mathbf{r}'$$

where $n, n' \leq n_{\max}$

Betzinger *et al., Phys. Rev. B* 81, 195117 (2010); H. Jiang *et al.,Comp. Phys. Comm.* 184, 348–366 (2013)

Hybrid functionals in **exciting**

NL matrix elements

$$V^{\mathrm{NL}}_{\mathrm{x},nn'}(\mathbf{k}) = -\sum_{n''}^{\mathrm{occ}} \sum_{\mathbf{k}'}^{\mathrm{BZ}} \int\int \frac{\varphi^*_{n\mathbf{k}}(\mathbf{r})\varphi_{n''\mathbf{k}'}(\mathbf{r})\varphi^*_{n''\mathbf{k}'}(\mathbf{r}')\varphi_{n'\mathbf{k}}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}d\mathbf{r}'$$

where $n, n' \leq n_{\max}$

6-dim integral

Betzinger *et al., Phys. Rev. B* 81, 195117 (2010); H. Jiang *et al.,Comp. Phys. Comm.* 184, 348–366 (2013)

Hybrid functionals in **exciting**

NL matrix elements

$$V_{\mathrm{x},nn'}^{\mathrm{NL}}(\mathbf{k}) = -\sum_{n''}^{\mathrm{occ}} \sum_{\mathbf{k}'}^{\mathrm{BZ}} \int\int \frac{\varphi_{n\mathbf{k}}^{*}(\mathbf{r})\varphi_{n''\mathbf{k}'}(\mathbf{r})\varphi_{n''\mathbf{k}'}^{*}(\mathbf{r}')\varphi_{n'\mathbf{k}}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}d\mathbf{r}'$$

where $n, n' \leq n_{\max}$

6-dim integral

Mixed product basis (MPB)

Betzinger *et al., Phys. Rev. B* 81, 195117 (2010); H. Jiang *et al.,Comp. Phys. Comm.* 184, 348–366 (2013)

Hybrid functionals in **exciting**

$$\varphi^{*}_{n\mathbf{k}}(\mathbf{r})\varphi_{n'\mathbf{k}-\mathbf{q}}(\mathbf{r}) = \sum_{I} M^{I}_{nn'}(\mathbf{k},\mathbf{k}-\mathbf{q})\chi^{\mathbf{q}}_{I}(\mathbf{r})$$

$$\{\chi^{\mathbf{q}}_{I}(\mathbf{r})\} \equiv \{\gamma^{\mathbf{q}}_{\alpha lm}(\mathbf{r}), P^{\mathbf{q}}_{I}(\mathbf{r})\}$$

Betzinger *et al., Phys. Rev. B* 81, 195117 (2010); H. Jiang *et al.,Comp. Phys. Comm.* 184, 348–366 (2013)

Hybrid functionals in **exciting**

$$\varphi^{*}_{n\mathbf{k}}(\mathbf{r})\varphi_{n'\mathbf{k}-\mathbf{q}}(\mathbf{r}) = \sum_{I} M^{I}_{nn'}(\mathbf{k},\mathbf{k}-\mathbf{q})\chi^{\mathbf{q}}_{I}(\mathbf{r})$$

$$\{\chi^{\mathbf{q}}_{I}(\mathbf{r})\} \equiv \{\gamma^{\mathbf{q}}_{\alpha lm}(\mathbf{r}), P^{\mathbf{q}}_{I}(\mathbf{r})\}$$

$$\Rightarrow \quad V^{\mathrm{NL}}_{\mathrm{x},nn'}(\mathbf{k}) = -\sum_{n''}^{\mathrm{occ}} \sum_{\mathbf{k}}^{\mathrm{BZ}} \sum_{IJ} [M^{I}_{nn''}(\mathbf{k},\mathbf{k}-\mathbf{q})]^{*} v_{IJ}(\mathbf{q}) M^{J}_{n''n'}(\mathbf{k},\mathbf{k}-\mathbf{q})$$

Vector-matrix-vector product

Betzinger *et al., Phys. Rev. B* 81, 195117 (2010); H. Jiang *et al.,Comp. Phys. Comm.* 184, 348–366 (2013)

Hybrid functionals in **exciting**

$$\varphi^{*}_{n\mathbf{k}}(\mathbf{r})\varphi_{n'\mathbf{k}-\mathbf{q}}(\mathbf{r}) = \sum_{I} M^{I}_{nn'}(\mathbf{k},\mathbf{k}-\mathbf{q})\chi^{\mathbf{q}}_{I}(\mathbf{r}) \qquad \{\chi^{\mathbf{q}}_{I}(\mathbf{r})\} \equiv \{\gamma^{\mathbf{q}}_{\alpha lm}(\mathbf{r}), P^{\mathbf{q}}_{I}(\mathbf{r})\}$$

$$\Rightarrow \quad V^{\mathrm{NL}}_{\mathrm{x},nn'}(\mathbf{k}) = -\sum_{n''}^{\mathrm{occ}} \sum_{\mathbf{k}}^{\mathrm{BZ}} \sum_{IJ} [M^{I}_{nn''}(\mathbf{k},\mathbf{k}-\mathbf{q})]^{*} v_{IJ}(\mathbf{q}) M^{J}_{n''n'}(\mathbf{k},\mathbf{k}-\mathbf{q})$$

MPB coefficients: $$M^{I}_{nn'}(\mathbf{k},\mathbf{k}-\mathbf{q}) = \int_{\Omega} [\chi^{\mathbf{q}}_{I}(\mathbf{r})\varphi_{n\mathbf{k}}(\mathbf{r})]^{*}\varphi_{n'\mathbf{k}-\mathbf{q}}(\mathbf{r})d\mathbf{r}$$

Bare Coulomb potential: $$v_{IJ}(\mathbf{q}) = \int\int \frac{[\chi^{\mathbf{q}}_{I}(\mathbf{r})]^{*}\chi^{\mathbf{q}}_{J}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}d\mathbf{r}'$$

Betzinger *et al., Phys. Rev. B* 81, 195117 (2010); H. Jiang *et al.,Comp. Phys. Comm.* 184, 348–366 (2013)

Hybrid functionals in **exciting**

Generalized eigenvalue problem in **LAPW+lo** basis

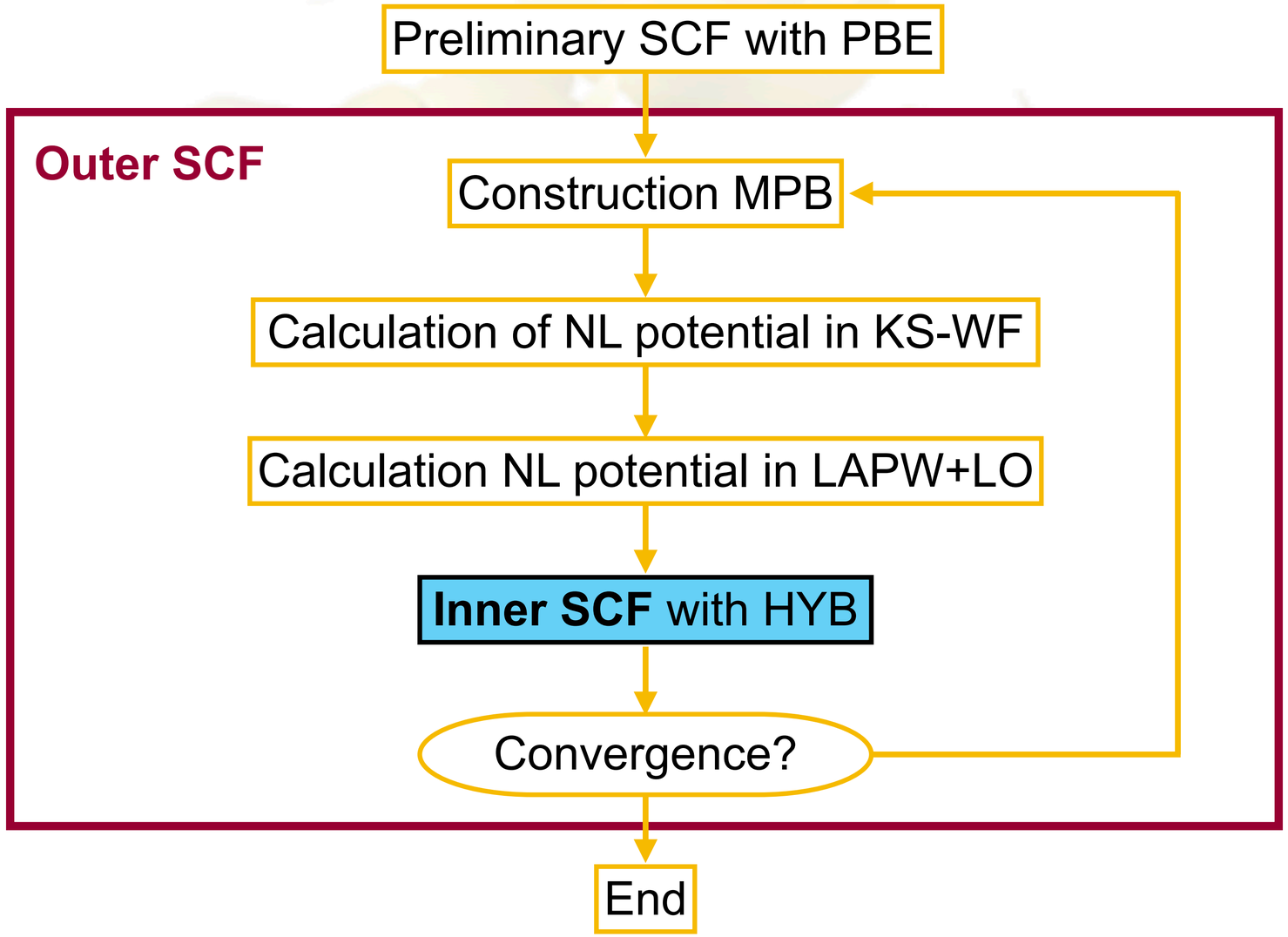
$$\sum_{\mathbf{G}'} [H_{\mathbf{G}\mathbf{G}'}(\mathrm{k}) + \alpha V^{\mathrm{NL}}_{\mathrm{x},\mathbf{G}\mathbf{G}'}(\mathbf{k})] C_{n\mathbf{G}'}(\mathbf{k}) = \varepsilon_{n\mathbf{k}} \sum_{\mathbf{G}'} S_{\mathbf{G}\mathbf{G}'}(\mathbf{k}) C_{n\mathbf{G}'}(\mathbf{k})$$

$$V^{\mathrm{NL}}_{\mathrm{x},\mathbf{G}\mathbf{G}'}(\mathbf{k}) = \sum_{nn'} \left[\sum_{\mathbf{G}''} S^{*}_{\mathbf{G}\mathbf{G}''}(\mathbf{k}) C_{n\mathbf{G}''}(\mathbf{k}) \right] V^{\mathrm{NL}}_{\mathrm{x},nn'}(\mathbf{k}) \left[\sum_{\mathbf{G}''} C^{*}_{n'\mathbf{G}''}(\mathbf{k}) S_{\mathbf{G}''\mathbf{G}'}(\mathbf{k}) \right]$$

where $n, n' \leq n_{\max}$

Betzinger *et al., Phys. Rev. B* 81, 195117 (2010); H. Jiang *et al.,Comp. Phys. Comm.* 184, 348–366 (2013)

Nested hybrid functionals SCF loop



Nested hybrid functionals SCF loop

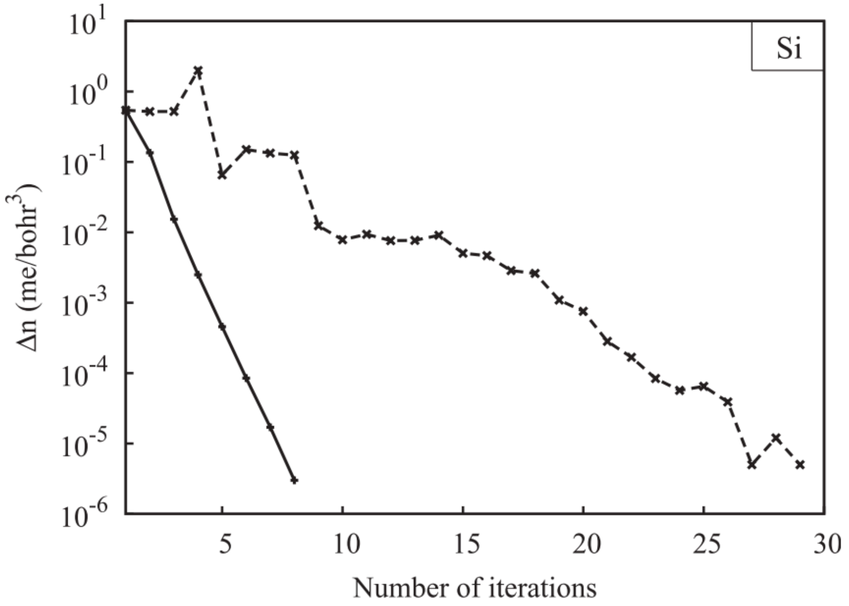


FIG. 3. Convergence behavior of the electron density for Si in a self-consistent-field cycle. The solid and dashed curves correspond to calculations with and without the nested density convergence scheme (see text).

Betzinger *et al., Phys. Rev. B* 81, 195117 (2010)

HSE06

$$E_{xc}^{HSE06} = E_{xc}^{PBE} + \alpha\left[E_{x}^{NL,SR}(\omega) - E_{x}^{PBE,SR}(\omega)\right]$$

$$\alpha = 0.25, \quad \omega = 0.11\ a_0^{-1}$$

$$v(r) = v^{SR}(r) + v^{LR}(r) = \frac{\mathrm{erfc}(\omega r)}{r} + \frac{\mathrm{erf}(\omega r)}{r}$$

Schlipf *et al., Phys. Rev. B* **84**, 125142 (2011)

HSE06

$$E_{xc}^{HSE06} = E_{xc}^{PBE} + \alpha\left[E_{x}^{NL,SR}(\omega) - E_{x}^{PBE,SR}(\omega)\right]$$

$$\alpha = 0.25, \quad \omega = 0.11\ a_0^{-1}$$

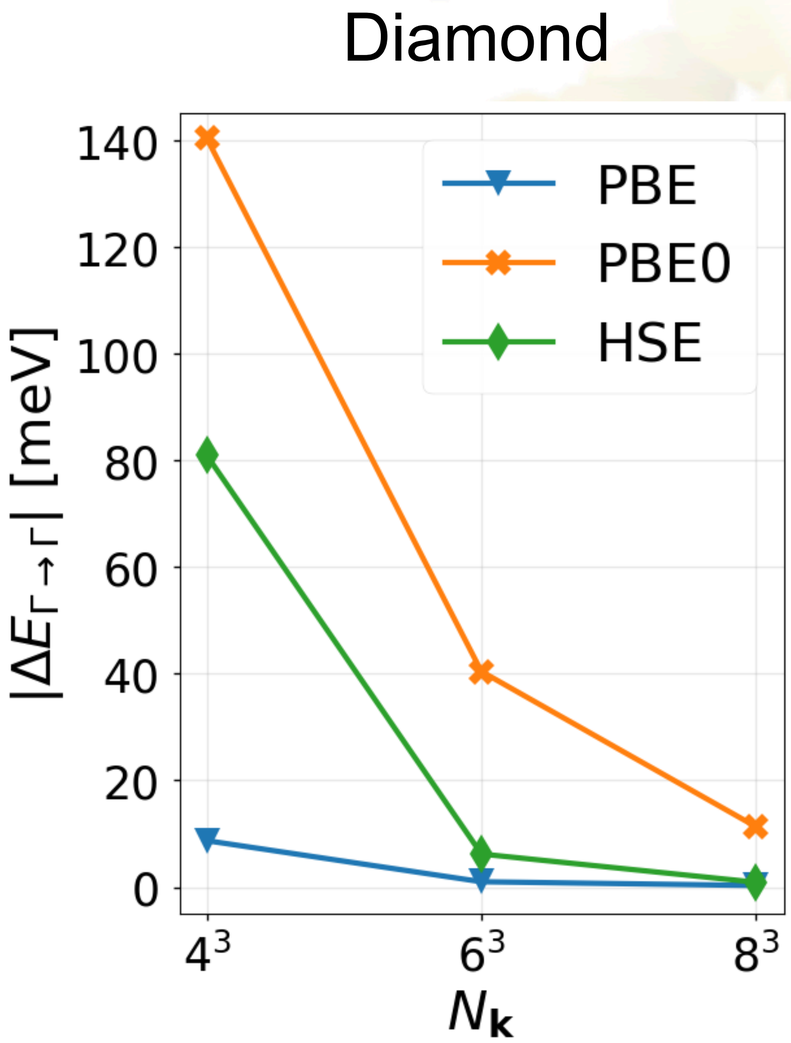
$$v(r) = v^{SR}(r) + v^{LR}(r) = \frac{\mathrm{erfc}(\omega r)}{r} + \frac{\mathrm{erf}(\omega r)}{r}$$

$$V_{x,nn'}^{NL,SR}(\mathbf{k}) = -\sum_{n''}^{occ}\sum_{\mathbf{k}}^{BZ}\sum_{IJ}[M_{nn''}^{I}(\mathbf{k},\mathbf{k}-\mathbf{q})]^{*} v_{IJ}^{SR}(\mathbf{q}) M_{n''n'}^{J}(\mathbf{k},\mathbf{k}-\mathbf{q})$$

$$v_{IJ}^{SR}(\mathbf{q}) = v_{IJ}(\mathbf{q}) - v_{IJ}^{LR}(\mathbf{q})$$

Schlipf *et al., Phys. Rev. B* **84**, 125142 (2011)

PBE0 vs HSE: k-points convergence



Computed with respect to $N_\mathbf{k} = 10^3$

From tutorial **Hybrid Functional Calculations**

Basic input & output

Basic input & output

PBE0

```
<input>

<title>Diamond PBE0</title>

...

   <groundstate
      ngridk="4 4 4"
      rgkmax="5.0"
      nempty="20"
      xctype="HYB_PBE0">
      <Hybrid
         excoeff="0.25" />
   </groundstate>

</input>
```

From tutorial **Hybrid Functional Calculations**

Basic input & output

PBE0

```
<input>

<title>Diamond PBE0</title>

...

   <groundstate
      ngridk="4 4 4"
      rgkmax="5.0"
      nempty="20"
      xctype="HYB_PBE0">
      <Hybrid
         excoeff="0.25" />
   </groundstate>

</input>
```

Functional name with prefix **HYB**

Element to specify hybrids parameters

From tutorial **Hybrid Functional Calculations**

Basic input & output

PBE0

```
<input>

<title>Diamond PBE0</title>

...

   <groundstate
      ngridk="4 4 4"
      rgkmax="5.0"
      nempty="20"
      xctype="HYB_PBE0">
      <Hybrid
         excoeff="0.25" />
   </groundstate>

</input>
```

$\alpha = 0.25$ default value

From tutorial **Hybrid Functional Calculations**

Basic input & output

PBE0

```
<input>

<title>Diamond PBE0</title>

...

   <groundstate
      ngridk="4 4 4"
      rgkmax="5.0"
      nempty="20"
      xctype="HYB_PBE0">
      <Hybrid
         excoeff="0.25" />
   </groundstate>

</input>
```

Number of unoccupied states
convergence parameter $(n, n' \leq n_{\max})$

From tutorial **Hybrid Functional Calculations**

Basic input & output

PBE0

```
<input>

<title>Diamond PBE0</title>

...

   <groundstate
      ngridk="4 4 4"
      rgkmax="5.0"
      nempty="20"
      xctype="HYB_PBE0">
      <Hybrid
         excoeff="0.25" />
   </groundstate>

</input>
```

HSE06

```
<input>

<title>Diamond HSE</title>

...

   <groundstate
      ngridk="4 4 4"
      rgkmax="5.0"
      nempty="20"
      xctype="HYB_HSE">
      <Hybrid
         excoeff="0.25"
         omega="0.11" />
   </groundstate>

</input>
```

$\omega = 0.11 a_0^{-1}$
default value

From tutorial **Hybrid Functional Calculations**

Basic input & output

INFO.OUT

```
********************************************************************************
* Hybrids module started
********************************************************************************

 Performing PBE self-consistent run
 Storing STATE_PBE.OUT

+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+ Hybrids iteration number :    1
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

...

+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Convergence target is reached
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+ Hybrids module stopped
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

Preliminary self consistent cycle with PBE

Iteration of the **outer** self-consistent cycle

Iteration **inner** self-consistent cycle hidden in INFO.OUT

From tutorial **Hybrid Functional Calculations**

Advanced input & output

Advanced input & output

```
<input>

<title>PbI2 HSE</title>

...

   <groundstate
      ngridk="3 3 2"
      rgkmax="8.0"
      nempty="280"
      xctype="HYB_HSE"
      outputlevel="high">
      <Hybrid
         excoeff="0.25"
         omega="0.11"
         mblksiz="32"
         lmaxmb="3"
         gmb="1"/>
   </groundstate>

</input>
```

INFO.OUT

```
Info(calc_vxnl):
   mdim, nblk, mblksiz:      151        5       32
   ---> rank, ikp, iq =        0        1        6
   locmatsiz, ngk, matsiz, mbsiz:    1111      298     1409     1409
   iblk, mstart, mend, size(minm) (Mb):        1        1       32         209.84
   iblk, mstart, mend, size(minm) (Mb):        2       33       64         209.84
   iblk, mstart, mend, size(minm) (Mb):        3       65       96         209.84
   iblk, mstart, mend, size(minm) (Mb):        4       97      128         209.84
   iblk, mstart, mend, size(minm) (Mb):        5      129      151         150.82
```

```
CPU time for vxnl (seconds)                   :      1220.24
CPU time for vnlmat (seconds)                 :         0.15
CPU time for scf_cycle (seconds)              :       172.68
```

Advanced input & output

```
<input>

<title>PbI2 HSE</title>

...

   <groundstate
      ngridk="3 3 2"
      rgkmax="8.0"
      nempty="280"
      xctype="HYB_HSE"
      outputlevel="high">
      <Hybrid
         excoeff="0.25"
         omega="0.11"
         mblksiz="32"
         lmaxmb="3"
         gmb="1" />
   </groundstate>

</input>
```

INFO.OUT

```
Info(calc_vxnl):
   mdim, nblk, mblksiz:       151         5        32
   ---> rank, ikp, iq =         0         1         6
   locmatsiz  ngk  matsiz, mbsiz:      1111       298      1409      1409
   iblk, mstart, mend, size(minm) (Mb):         1         1        32       209.84
   iblk, mstart, mend, size(minm) (Mb):         2        33        64       209.84
   iblk, mstart, mend, size(minm) (Mb):         3        65        96       209.84
   iblk, mstart, mend, size(minm) (Mb):         4        97       128       209.84
   iblk, mstart, mend, size(minm) (Mb):         5       129       151       150.82
```

matsiz, mbsiz = dimension of the mixed product basis

$$\{\chi_I^{\mathbf{q}}(\mathbf{r})\} \equiv \{\gamma_{\alpha lm}^{\mathbf{q}}(\mathbf{r}), P_I^{\mathbf{q}}(\mathbf{r})\}$$

lmaxmb: max. angular momentum in the construction of the MT part

gmb: interstitial-PW energy cutoff in the construction of the I part

Advanced input & output

```
<input>

<title>PbI2 HSE</title>

...

   <groundstate
      ngridk="3 3 2"
      rgkmax="8.0"
      nempty="280"
      xctype="HYB_HSE"
      outputlevel="high">
      <Hybrid
         excoeff="0.25"
         omega="0.11"
         mblksiz="32"
         lmaxmb="3"
         gmb="1"/>
   </groundstate>

</input>
```

INFO.OUT

```
Info(calc_vxnl):
   mdim, nblk, mblksiz:          151        5       32
    ---> rank, ikp, iq =           0        1        6
    locmatsiz, ngk, matsiz, mbsiz:    1111      298     1409     1409
    iblk, mstart, mend, size(minm) (Mb):        1        1       32      209.84
    iblk, mstart, mend, size(minm) (Mb):        2       33       64      209.84
    iblk, mstart, mend, size(minm) (Mb):        3       65       96      209.84
    iblk, mstart, mend, size(minm) (Mb):        4       97      128      209.84
    iblk, mstart, mend, size(minm) (Mb):        5      129      151      150.82
```

mdim: number of occupied states included core states

nblk: number of blocks

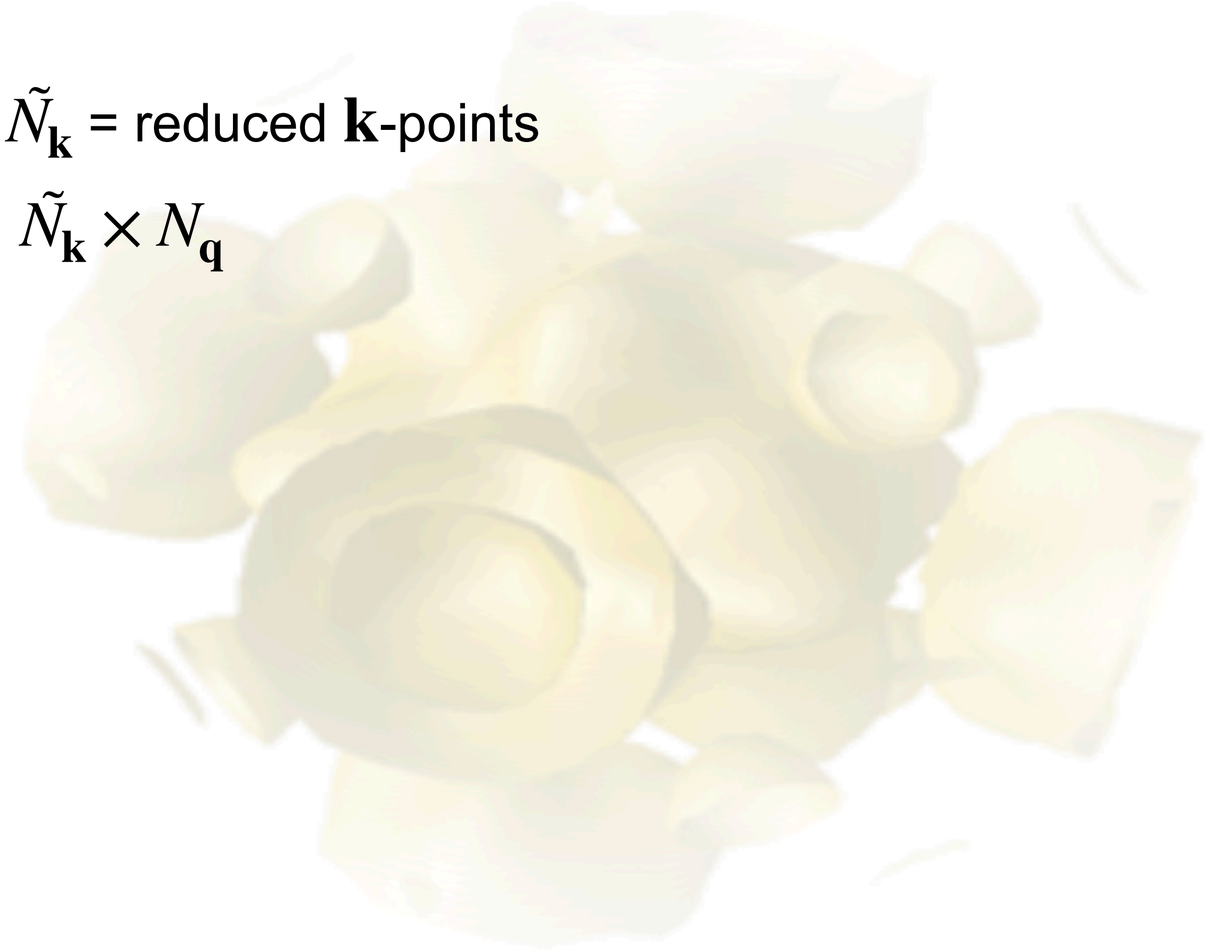
$$V_{\mathrm{x},nn'}^{\mathrm{NL}}(\mathbf{k}) = -\sum_{n''}^{\mathrm{occ}} \sum_{\mathbf{k}}^{\mathrm{BZ}} \sum_{IJ} [M_{nn''}^{I}(\mathbf{k}, \mathbf{k}-\mathbf{q})]^{*} v_{IJ}(\mathbf{q}) M_{n''n'}^{J}(\mathbf{k}, \mathbf{k}-\mathbf{q})$$

MPI parallelization

MPI parallelization

Inner cycle: $\tilde{N}_{\mathbf{k}}$ = reduced $\mathbf{k}$-points

NL potential: $\tilde{N}_{\mathbf{k}} \times N_{\mathbf{q}}$



MPI parallelization

Inner cycle: $\tilde{N}_{\mathbf{k}}$ = reduced $\mathbf{k}$-points

NL potential: $\tilde{N}_{\mathbf{k}} \times N_{\mathbf{q}}$

PbI_2

$N_{\mathbf{k}} = 3 \times 3 \times 2$:

$6\,\tilde{N}_{\mathbf{k}} \times 18\,N_{\mathbf{q}} = 108$

MPI parallelization

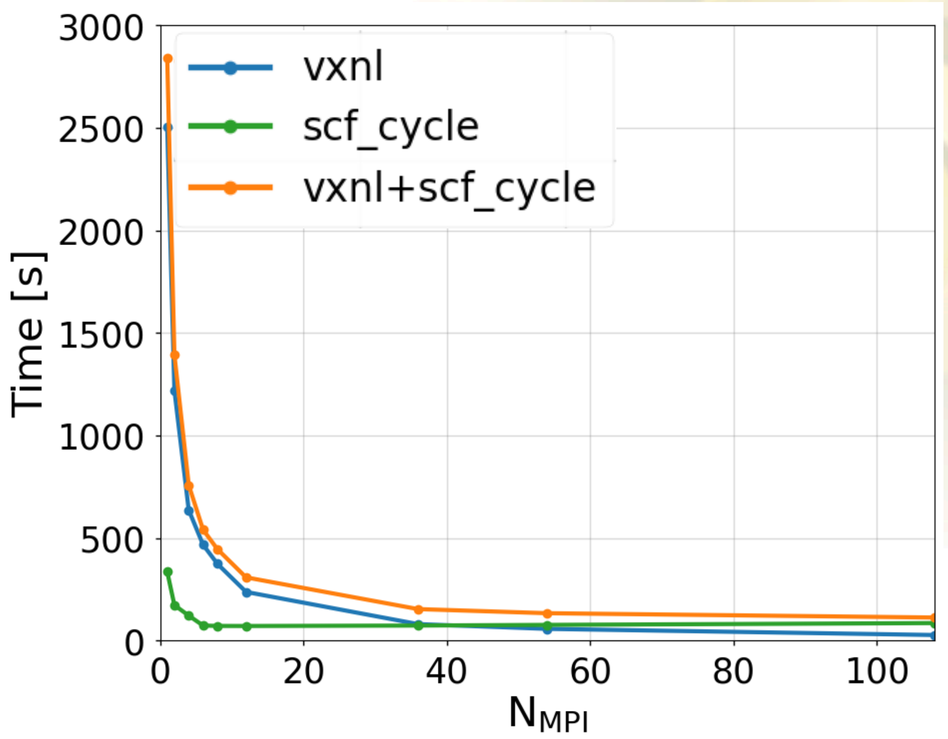
Inner cycle: $\tilde{N}_{\mathbf{k}}$ = reduced $\mathbf{k}$-points

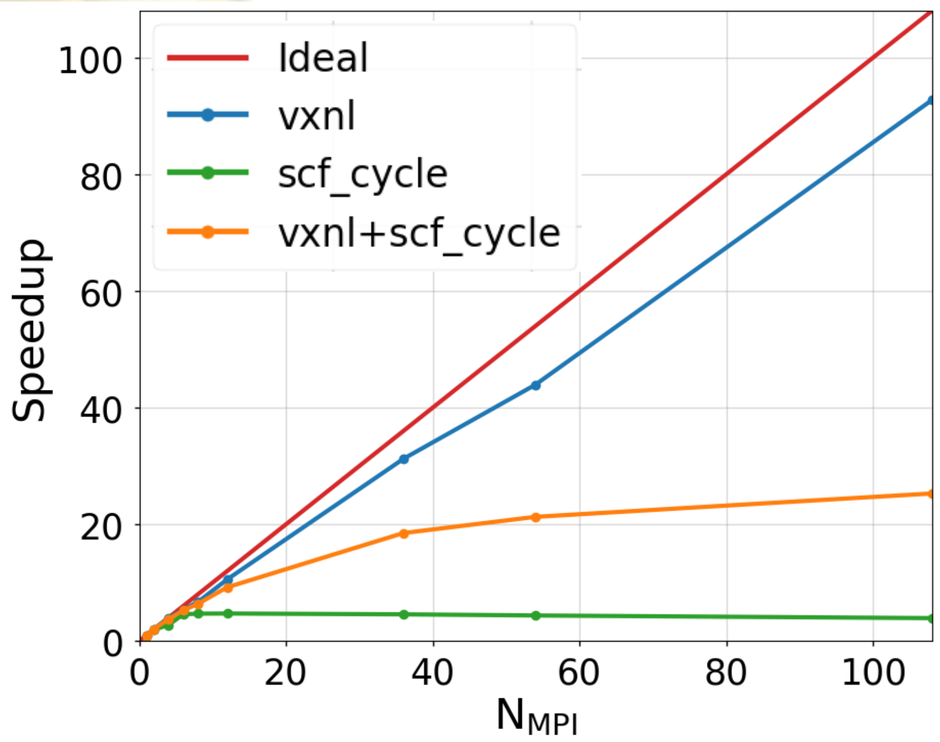
NL potential: $\tilde{N}_{\mathbf{k}} \times N_{\mathbf{q}}$

PbI_2

$N_{\mathbf{k}} = 3 \times 3 \times 2$:

$6\,\tilde{N}_{\mathbf{k}} \times 18\,N_{\mathbf{q}} = 108$





HSE06 singularity treatment

$$v_{ij}^{SR,s} = v_{ij}^{s} - v_{ij}^{LR,s} = \lim_{\mathbf{q}+\mathbf{G}\to\mathbf{0}} \frac{4\pi}{|\mathbf{q}+\mathbf{G}|^2}\left(1 - e^{-|\mathbf{q}+\mathbf{G}|^2/4\omega^2}\right) = \frac{\pi}{\omega^2}$$

Schlipf *et al., Phys. Rev. B* **84**, 125142 (2011); Vona *et al., Adv. Theory Simul.* **5**, 2100496 (2022)

HSE06 singularity treatment

$$v_{ij}^{SR,s} = v_{ij}^{s} - v_{ij}^{LR,s} = \lim_{\mathbf{q}+\mathbf{G}\to\mathbf{0}} \frac{4\pi}{|\mathbf{q}+\mathbf{G}|^2}\left(1 - e^{-|\mathbf{q}+\mathbf{G}|^2/4\omega^2}\right) = \frac{\pi}{\omega^2}$$

$$I_s = \frac{1}{V_\mathbf{k}} \int_{V_\mathbf{k}} d\mathbf{q} \frac{4\pi}{q^2}\left(1 - e^{-q^2/4\omega^2}\right) = \frac{16\pi^2}{V_\mathbf{k}} \int_0^{R_\mathbf{k}} dq \left(1 - e^{-q^2/4\omega^2}\right)$$

Schlipf *et al., Phys. Rev. B* **84**, 125142 (2011); Vona *et al., Adv. Theory Simul.* **5**, 2100496 (2022)

HSE06 singularity treatment

$$v_{ij}^{SR,s} = v_{ij}^{s} - v_{ij}^{LR,s} = \lim_{\mathbf{q}+\mathbf{G}\to\mathbf{0}} \frac{4\pi}{|\mathbf{q}+\mathbf{G}|^2}\left(1 - e^{-|\mathbf{q}+\mathbf{G}|^2/4\omega^2}\right) = \frac{\pi}{\omega^2}$$

$$I_s = \frac{1}{V_\mathbf{k}} \int_{V_\mathbf{k}} d\mathbf{q} \frac{4\pi}{q^2}\left(1 - e^{-q^2/4\omega^2}\right) = \frac{16\pi^2}{V_\mathbf{k}} \int_0^{R_\mathbf{k}} dq \left(1 - e^{-q^2/4\omega^2}\right)$$

Taylor expansion

$$I_s^T = \frac{\pi}{\omega^2}$$

Schlipf *et al., Phys. Rev. B* **84**, 125142 (2011); Vona *et al., Adv. Theory Simul.* **5**, 2100496 (2022)

HSE06 singularity treatment

$$v_{\mathrm{ij}}^{\mathrm{SR,s}} = v_{\mathrm{ij}}^{\mathrm{s}} - v_{\mathrm{ij}}^{\mathrm{LR,s}} = \lim_{\mathbf{q}+\mathbf{G}\to\mathbf{0}} \frac{4\pi}{|\mathbf{q}+\mathbf{G}|^2}\left(1 - \mathrm{e}^{-|\mathbf{q}+\mathbf{G}|^2/4\omega^2}\right) = \frac{\pi}{\omega^2}$$

$$I_{\mathrm{s}} = \frac{1}{V_{\mathbf{k}}}\int_{V_{\mathbf{k}}} \mathrm{d}\mathbf{q}\frac{4\pi}{q^2}\left(1 - \mathrm{e}^{-q^2/4\omega^2}\right) = \frac{16\pi^2}{V_{\mathbf{k}}}\int_0^{R_{\mathbf{k}}} \mathrm{d}q\left(1 - \mathrm{e}^{-q^2/4\omega^2}\right)$$

Taylor expansion

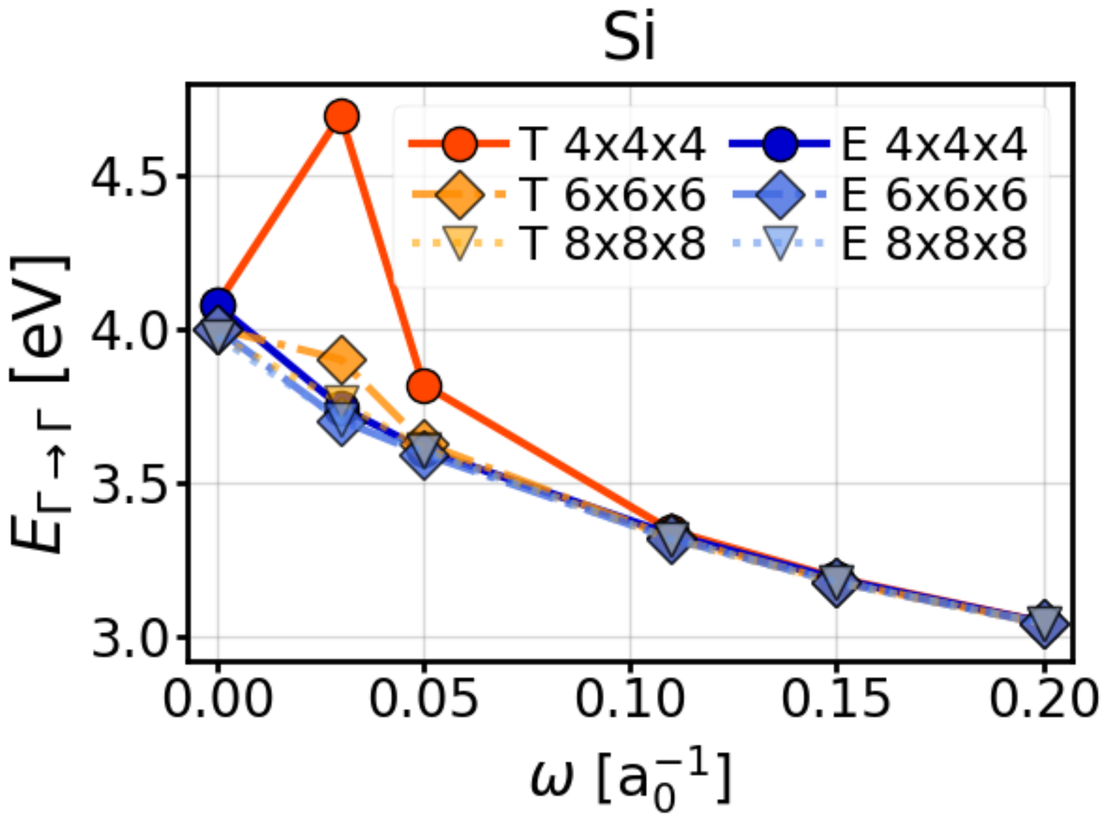
$$I_{\mathrm{s}}^{\mathrm{T}} = \frac{\pi}{\omega^2}$$

Exact integral solution

$$I_{\mathrm{s}}^{\mathrm{E}} = \frac{16\pi^2}{V_{\mathbf{k}}}\left(R_{\mathbf{k}} - \sqrt{\pi\omega^2}\,\mathrm{erf}\left(\sqrt{\frac{1}{4\omega^2}}\mathrm{R}_{\mathbf{k}}\right)\right)$$

Schlipf *et al., Phys. Rev. B* **84**, 125142 (2011); Vona *et al., Adv. Theory Simul.* **5**, 2100496 (2022)

HSE06 singularity treatment

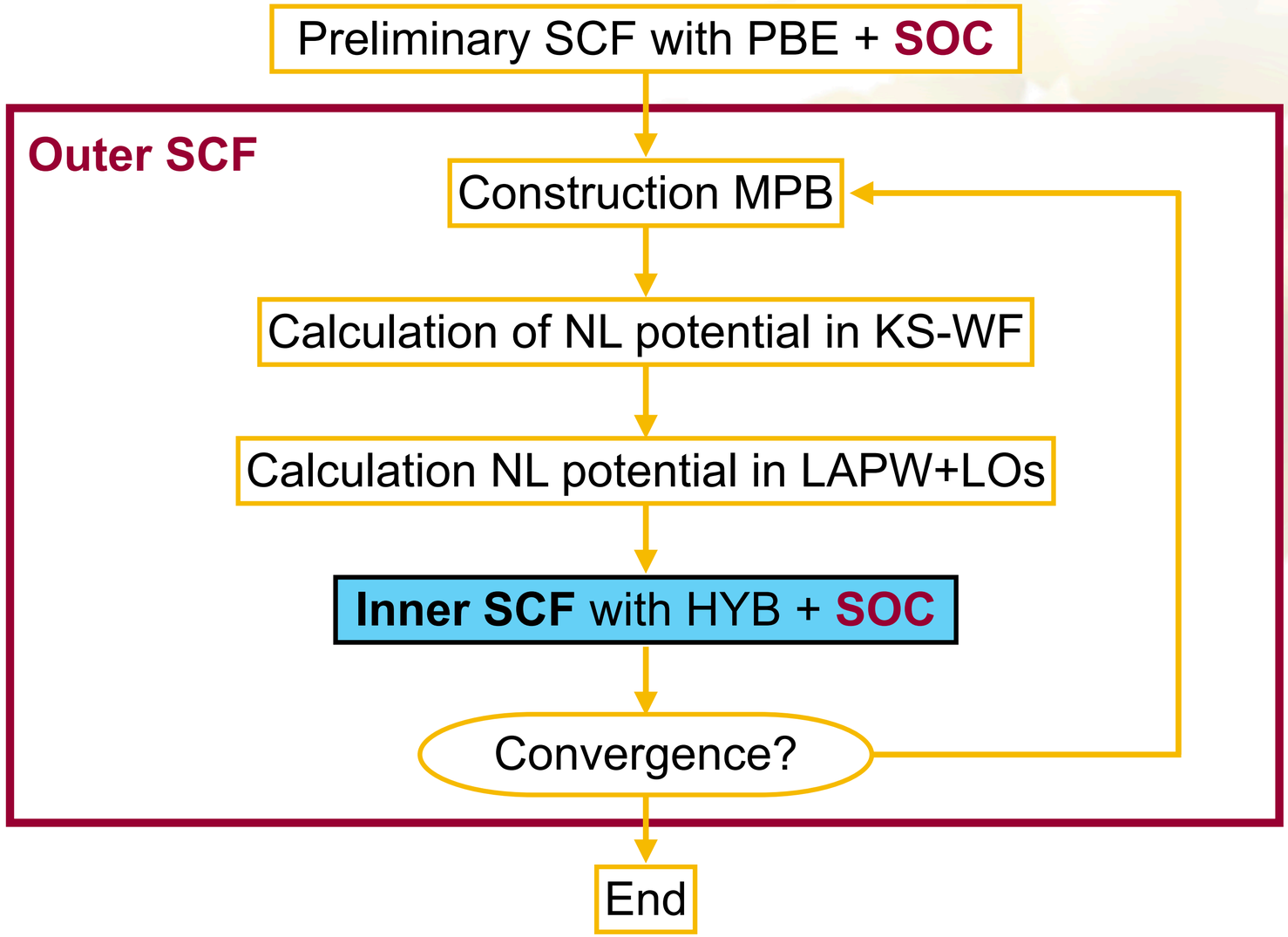


HSE06 singularity treatment

```
<input>

<title>Diamaond HSE</title>

...

  <groundstate
     ngridk="4 4 4"
     rgkmax="5.0"
     nempty="20"
     xctype="HYB_HSE"
     >
     <Hybrid
       excoeff="0.25"
       omega="0.11"
       HSEsingularity="Exact"/>
  </groundstate>

</input>
```

HSEsingularity="Taylor"
default method to compute the singularity integral

Hybrid functionals with SOC



SOC is evaluated through

second variation

Hybrid functionals with SOC

```
<input>

<title>PbI2 HSE</title>

...

   <groundstate
      ngridk="3 3 2"
      rgkmax="8.0"
      nempty="280"
      xctype="HYB_HSE">
      <spin
         spinorb="true"
         realspace="true"/>
      <Hybrid
         excoeff="0.25"
         omega="0.11"/>
   </groundstate>

</input>
```

Number of unoccupied states convergence parameter also for SOC

Spin element

Summary

- Overview of hybrid functionals implementation
- Input & output files
- Parallelization
- Singularity treatment in HSE
- SOC with hybrid functionals

Summary

- Overview of hybrid schema
- Input & output files
- Parallelization
- Singularity treatment in HSE
- SOC with hybrid functionals

Wannier functions interpolation for DOS and band structures

Summary

- Overview of hybrid schema
- Input & output files
- Parallelization
- Singularity treatment in HSE
- SOC with hybrid functionals

Wannier functions interpolation for DOS and band structures

Thank you!