Accurately predicting electron affinities with Koopmans spectral functionals

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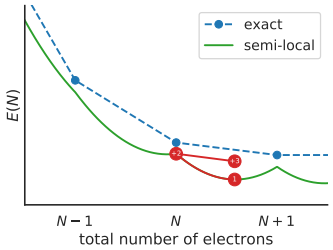
EPFL

Theory



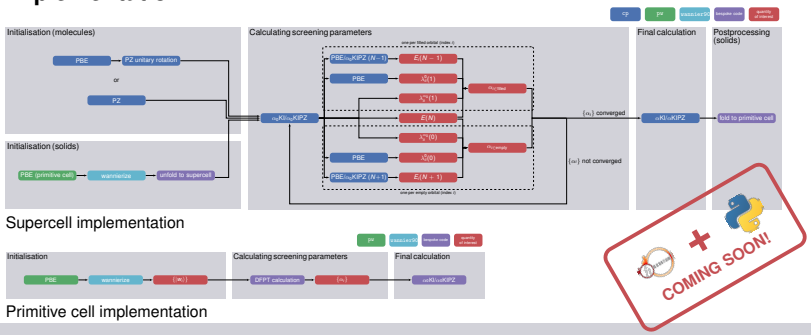
The goal:
$\varepsilon_i = \langle\varphi_i|H|\varphi_i\rangle = \partial E/\partial f_i$ independent of f_i

The functional:

$$E_{KC}[\rho, \{f_i\}, \{\alpha_i\}] = E_{DFT}[\rho] + \sum_i \alpha_i \left(- \int_0^{f_i} \varepsilon_i(f) df + f_i \int_0^1 \varepsilon_i(f) df \right)$$

Dabo *et al*, Phys. Rev. B 82, 115121
Borghi *et al*, Phys. Rev. B 90, 075135
Nguyen *et al*, Phys. Rev. X 8, 021051

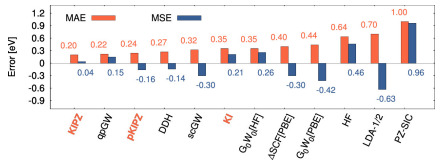
Implementation



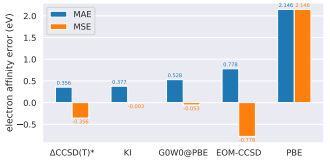
Supercell implementation

Primitive cell implementation

Results



Colonna *et al*, JCTC 2018, 14, 5, 25492557



Linscott *et al*, in prep.