



Center for Scientific Computing,
Theory and Data

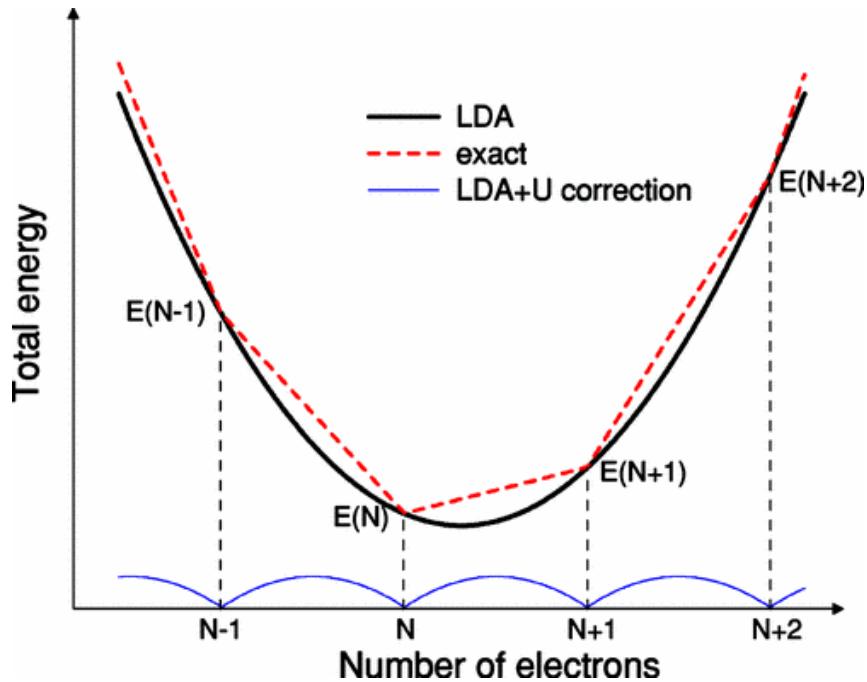
Are our corrections correct?

A provocative chat among friends

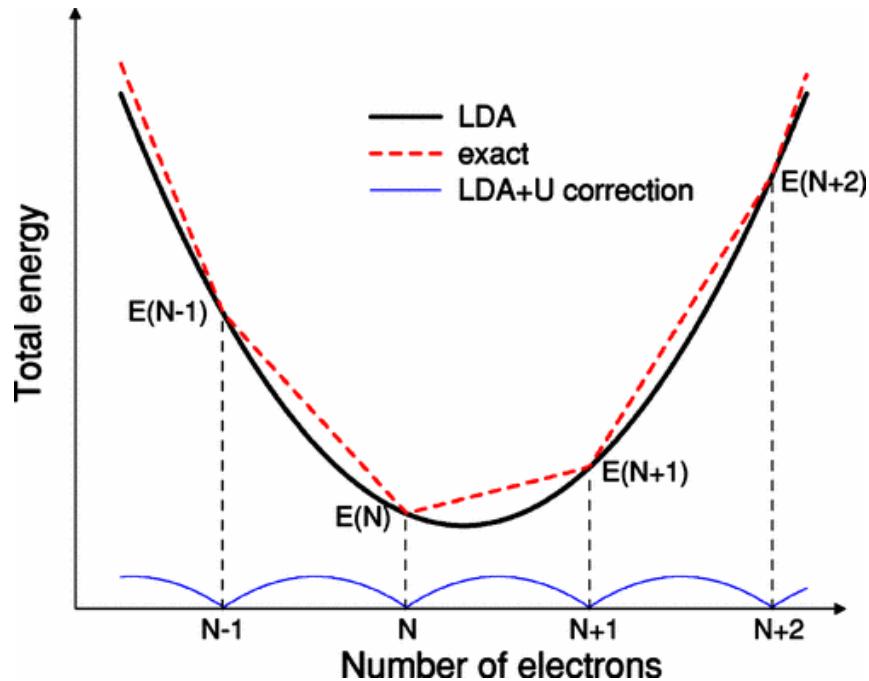
Edward Linscott

THEOS Group Meeting, 3 October 2024

Our starting point: piecewise linearity

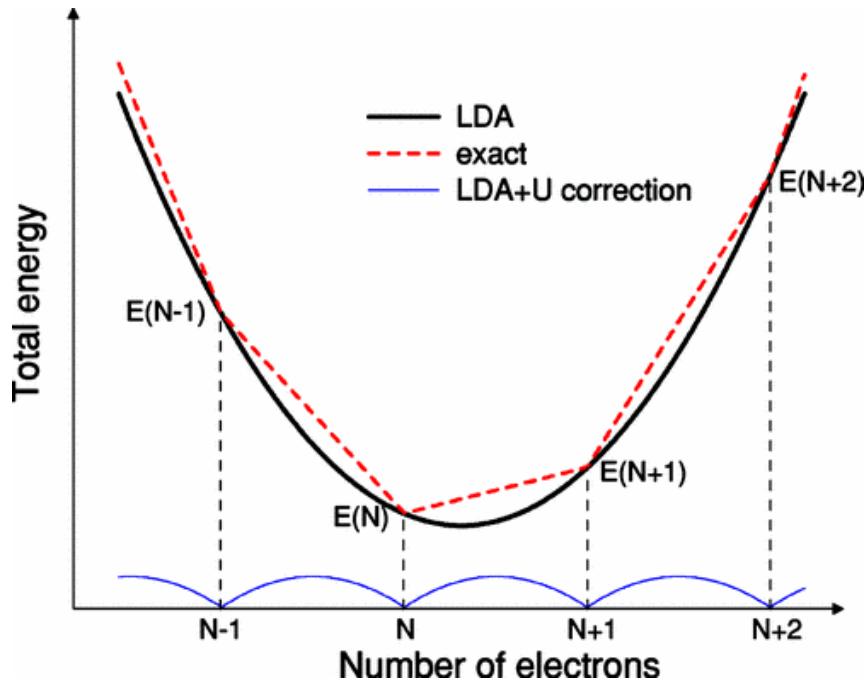


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This idea of piecewise linearity is central to a lot of what we do

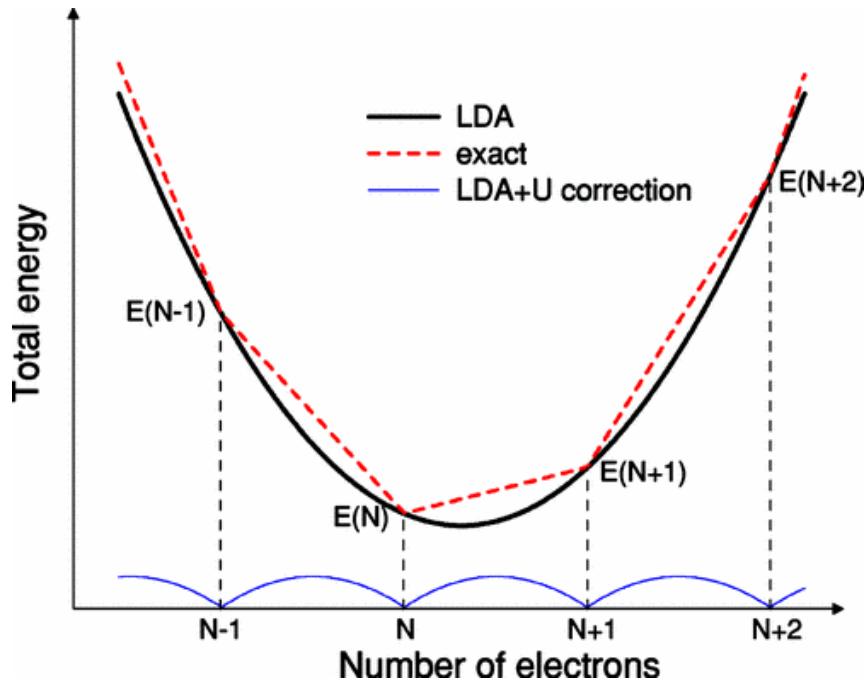
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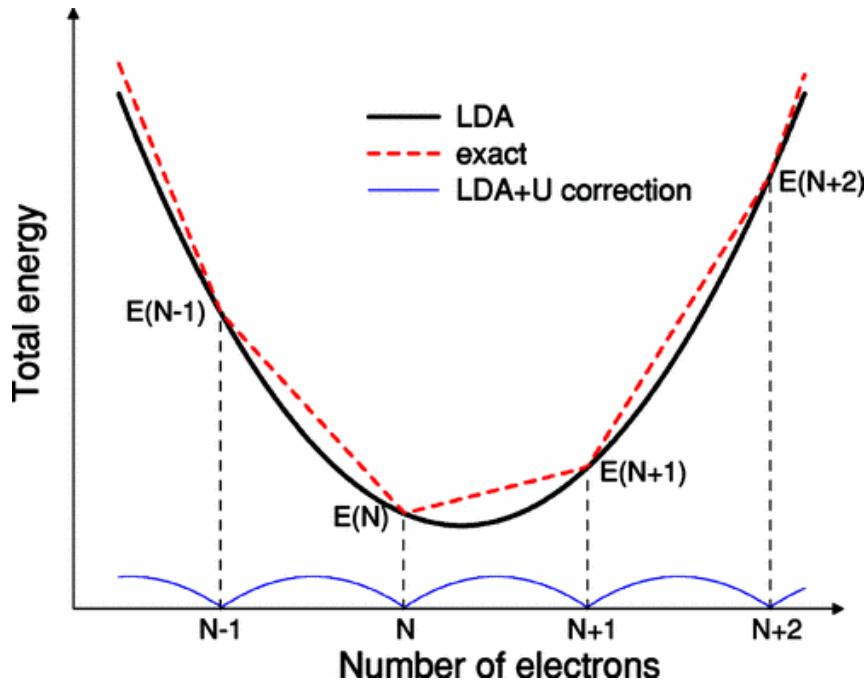
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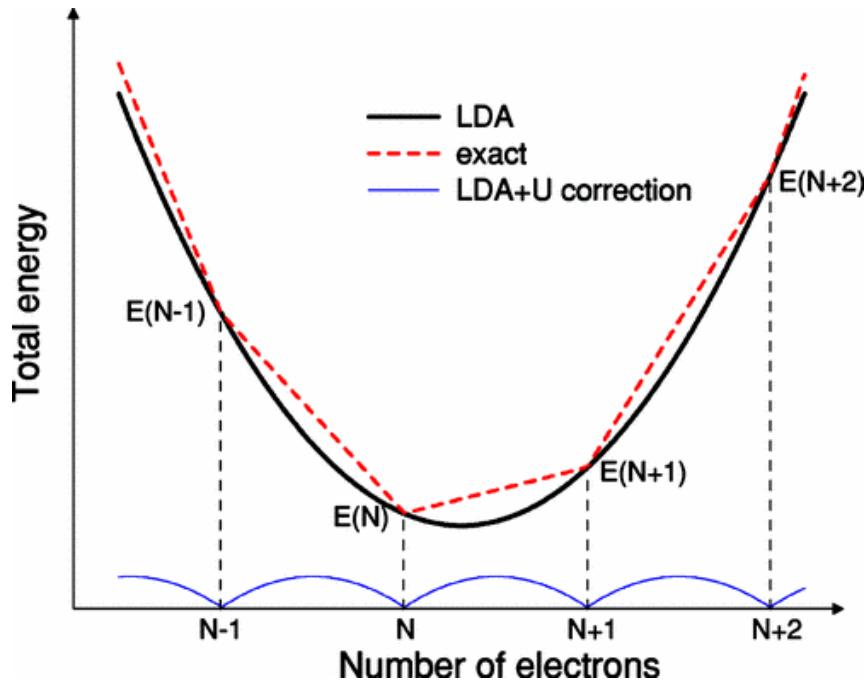
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- dynamical functionals
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- DFT+ U (and its + V and + J extensions)
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- dynamical functionals
- ...

Exact conditions

PWL

$$\frac{d^2 E}{dN^2} = 0$$

Generalised PWL

$$\Delta E_i = \varepsilon_i \iff \frac{d^2 E}{df_i^2} = 0$$

DFT+*U*

$$\begin{aligned}
 E_U &= \sum_{Imm'\sigma} \frac{U^I}{2} n_{mm'} (\delta_{m'm} - n_{m'm'}) \\
 &= \sum_{Ii\sigma} \frac{U^I}{2} \lambda_i^{I\sigma} (1 - \lambda_i^{I\sigma})
 \end{aligned}$$

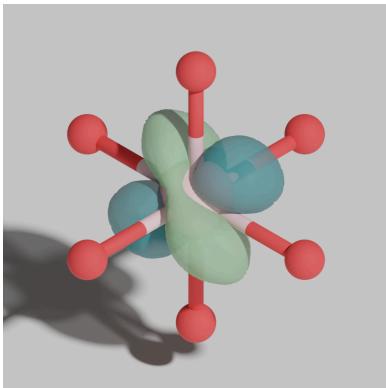
$$\begin{aligned}
 \hat{V}_U^\sigma &= \sum_{Imm'} \frac{U^I}{2} (\delta_{mm'} - 2n_{mm'}^{I\sigma}) |\varphi_m^{I\sigma}\rangle \langle \varphi_{m'}^{I\sigma}| \\
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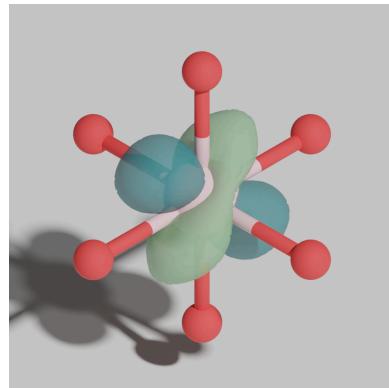
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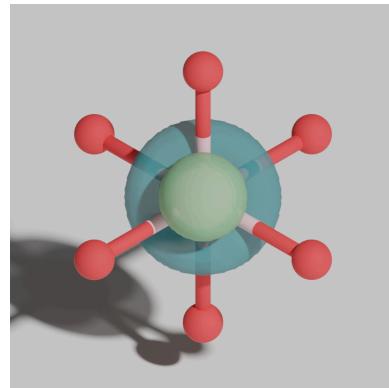
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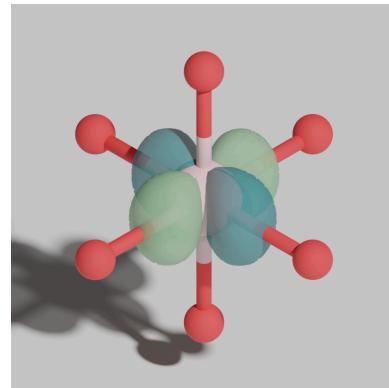
$$\lambda_1^{I\sigma} = 0.99$$



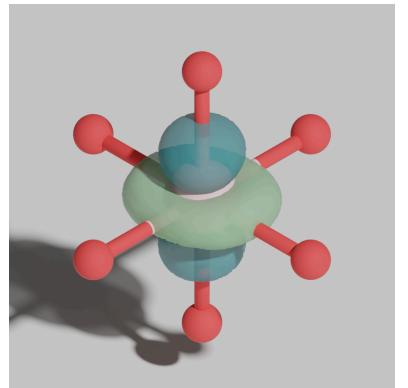
$$\lambda_2^{I\sigma} = 0.99$$



$$\lambda_3^{I\sigma} = 0.99$$



$$\lambda_4^{I\sigma} = 0.36$$



$$\lambda_5^{I\sigma} = 0.36$$

The link between PWL and DFT+ U is imperfect



¹A. Bajaj *et al.* *J. Chem. Phys.* **147**, 191101–191102 (2017)

The link between PWL and DFT+ U is imperfect

- corrects curvature with respect to $\lambda_i^{I\sigma}$ — local, not global curvature (N)¹
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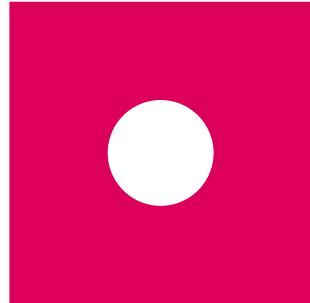
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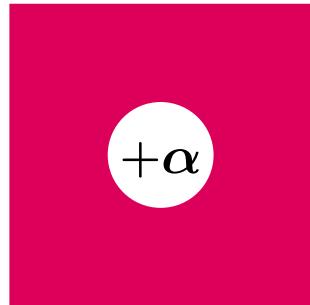
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 - frontier orbital argument; or
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- orbitals are *partially* determined by the user
- the recipe for calculating U via linear-response involves charge-conserving perturbations

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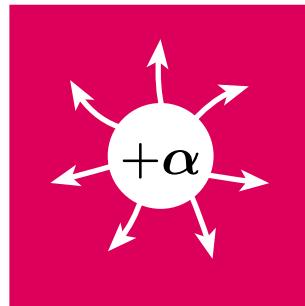
An alternative recipe



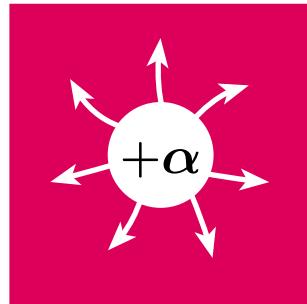
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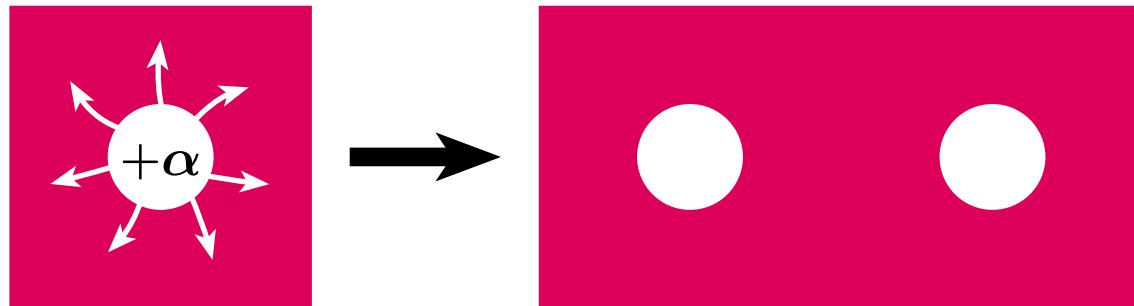


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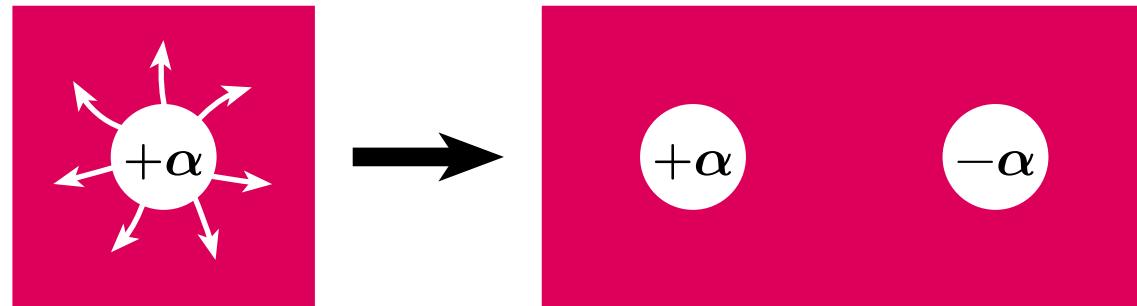
$$\Delta n \neq 0; \Delta N = 0$$

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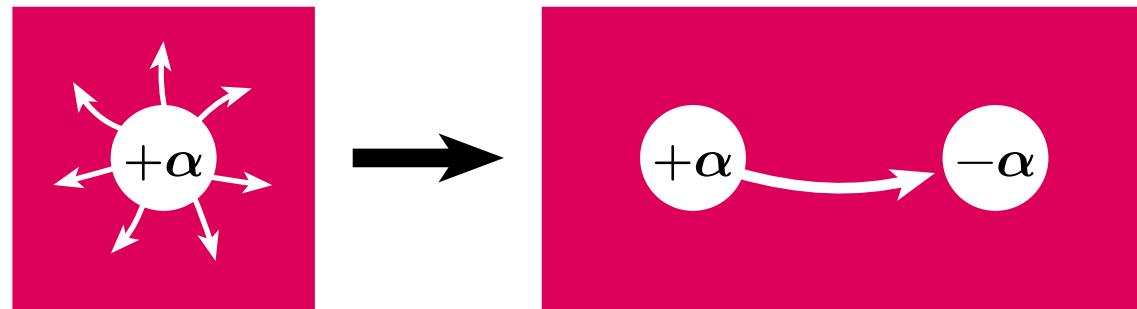
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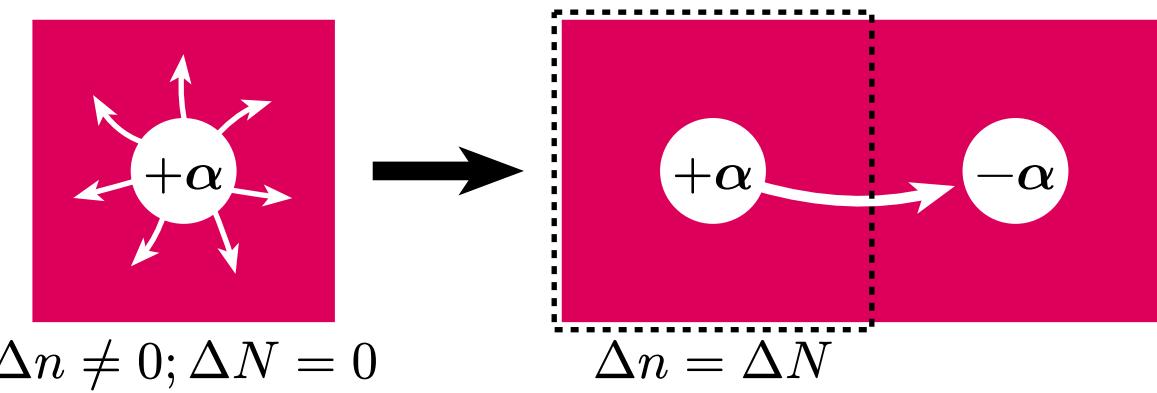
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DFT+ U + V

$$E_V = - \sum_{IJ}^* \frac{V^{IJ}}{2} \sum_{ij\sigma} n_{ij}^{IJ\sigma} n_{ij}^{JI\sigma} \quad \text{and} \quad \hat{V}_V^\sigma = - \sum_{IJ}^* V^{IJ} \sum_{ij} n_{ji}^{JI\sigma} |\varphi_i^{I\sigma}\rangle \langle \varphi_j^{J\sigma}|$$

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Harder to relate to PWL. For *s*-orbital Hubbard subspaces...

$$\frac{d^2 E_V}{dn^{IJ\sigma} dn^{JI\sigma}} = V^{IJ}$$

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cf. the $+V$ LR recipe $\chi^{IJ} = \frac{dn^{II}}{d\alpha^J}$ which relates to $\frac{d^2 E}{dn^{I\sigma} dn^{J\sigma}}$

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In lieu of PWL, we can resort to traditional arguments

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In lieu of PWL, we can resort to traditional arguments

But in *some* cases DFT+U+V results are better than DFT+U – how can we make sense of this?

Off-diagonal corrections as diagonal corrections

We have

$$\hat{V}_U^\sigma = \sum_{Ii} \frac{U^I}{2} (1 - 2\lambda_i^{I\sigma}) |\varphi_i^{I\sigma}\rangle \langle \varphi_i^{I\sigma}| \quad \text{and} \quad \hat{V}_V^\sigma = - \sum_{IJ}^* V^{IJ} \sum_{ij} n_{ji}^{JI\sigma} |\varphi_i^{I\sigma}\rangle \langle \varphi_j^{J\sigma}|$$

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It is simple to prove that

$$\hat{V}_U^\sigma + \hat{V}_V^\sigma = \sum_{Ii\sigma} \frac{U^I}{2} (1 - 2\lambda_i) |\tilde{\varphi}_i^{I\sigma}\rangle \langle \tilde{\varphi}_i^{I\sigma}|$$

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where we have the hybridised orbitals

$$|\tilde{\varphi}_i^{I\sigma}\rangle = |\varphi_i^{I\sigma}\rangle + \sum_J^* \sum_j c_{ij}^{IJ\sigma} |\varphi_j^{J\sigma}\rangle \quad c_{ij}^{IJ\sigma} = \frac{2V^{IJ} n_{ji}^{JI\sigma}}{U^J (1 - 2\lambda_j^{J\sigma}) - U^I (1 - 2\lambda_i^{I\sigma})}$$

Off-diagonal corrections as diagonal corrections



$$\hat{V}_{U+V}^{\sigma} = \sum_{Ii\sigma} \frac{U^I}{2} (1 - 2\lambda_i) |\tilde{\varphi}_i^{I\sigma}\rangle\langle\tilde{\varphi}_i^{I\sigma}| \quad |\tilde{\varphi}_i^{I\sigma}\rangle = |\varphi_i^{I\sigma}\rangle + \sum_J^* \sum_j c_{ij}^{IJ\sigma} |\varphi_j^{J\sigma}\rangle$$

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Off-diagonal corrections as diagonal corrections



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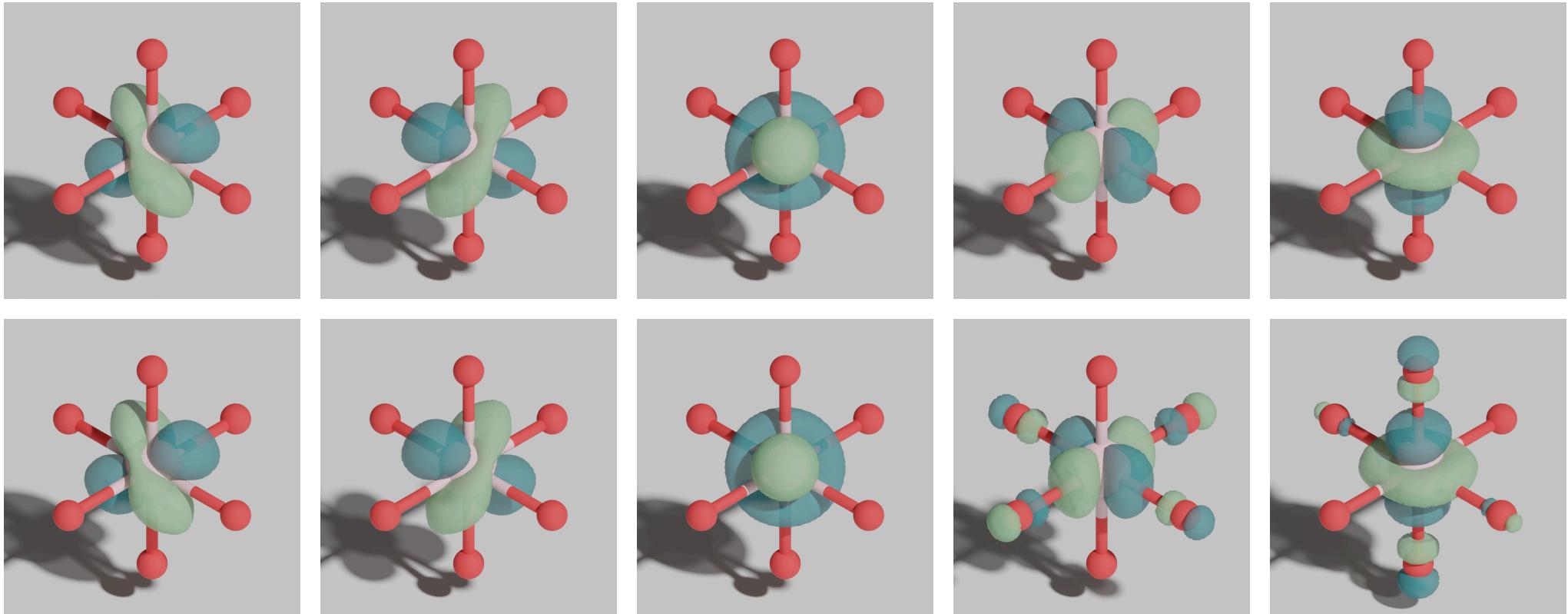
Off-diagonal corrections as diagonal corrections



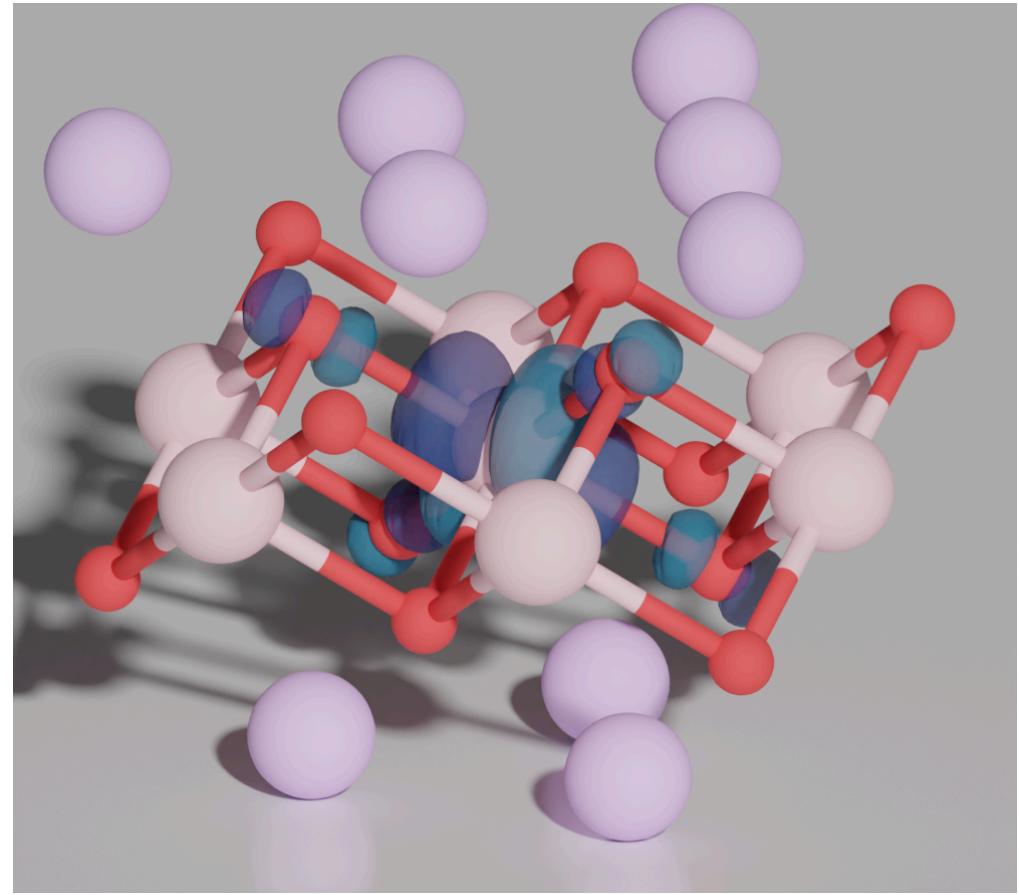
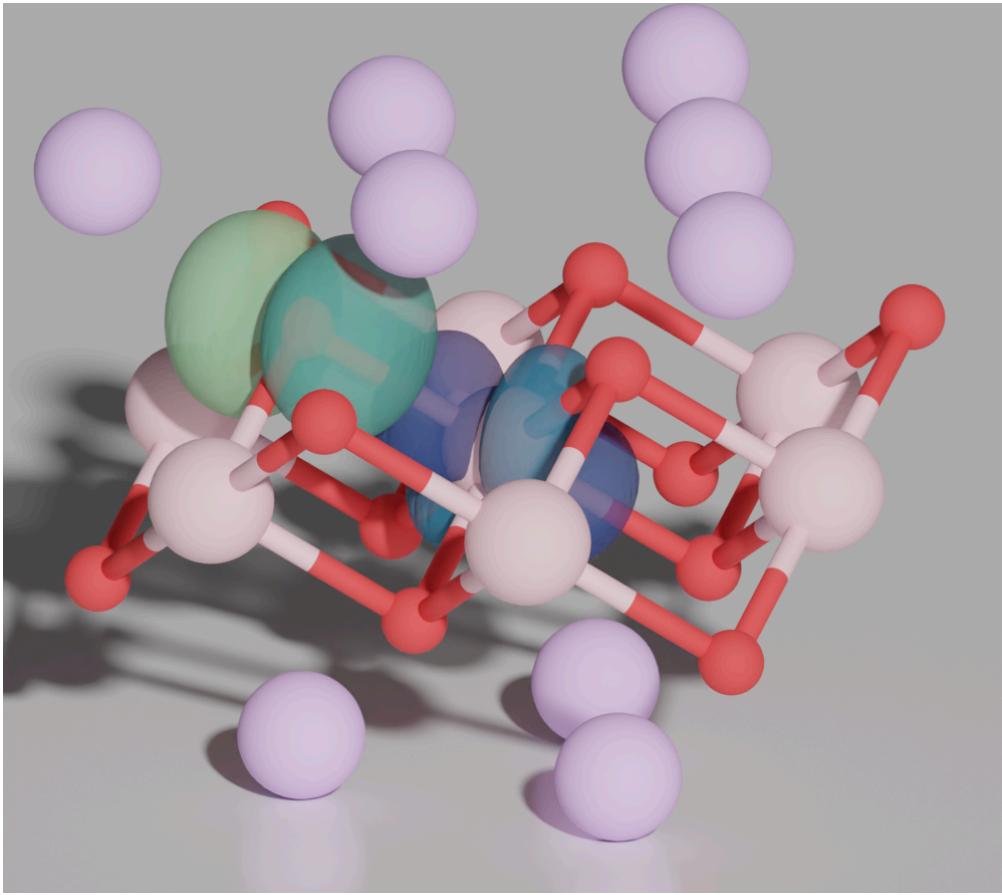
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- DFT+ $U+V$ is equivalent to DFT+ U using hybridised projectors!
- the degree of hybridisation ($c_{ij}^{IJ\sigma}$) depends on U , V , n_{ij}^{IJ}
- only valid in $U \gg V$ limit, not self-consistent
- PWL applies!

Off-diagonal corrections as diagonal corrections



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Ramifications for linear response



Suppose we now want to linearise E wrt the occupation of the hybridised orbitals

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Ramifications for linear response

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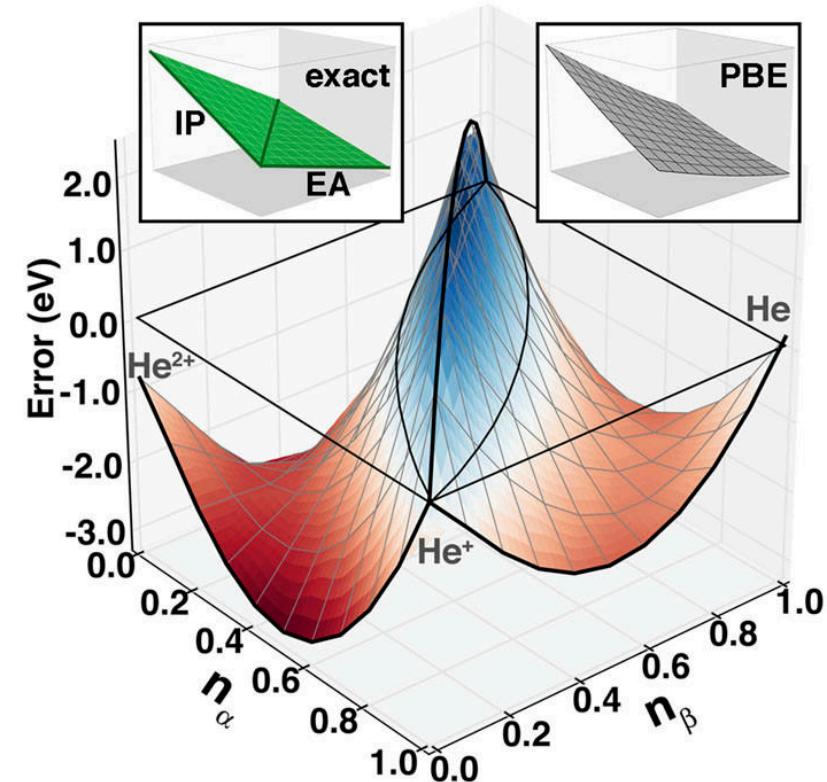
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We have terms that don't appear in conventional LR!

DFT+*U*+*J*

E should also be piecewise linear as a function of the magnetization¹

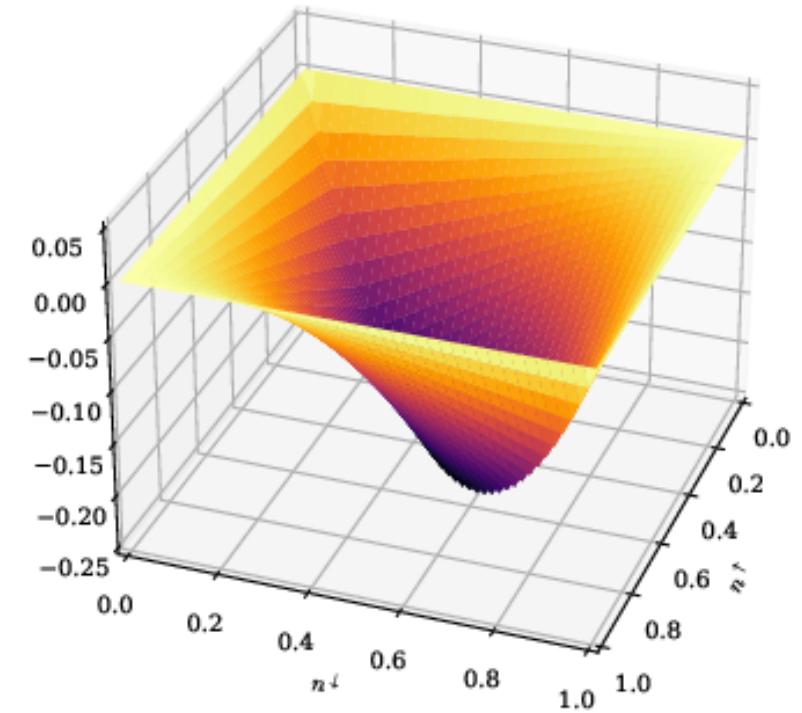
DFT typically gives an erroneous concave curvature²



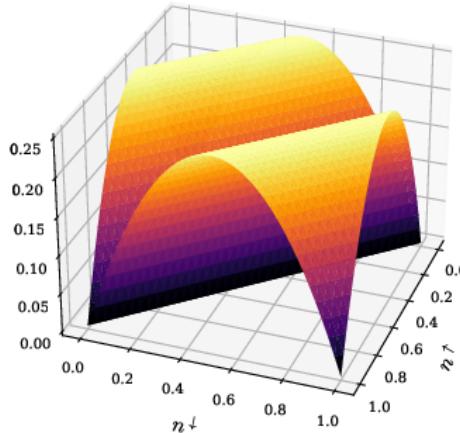
¹A. C. Burgess et al. *The Journal of Chemical Physics* **159**, 211102–211103 (2023)

²A. Bajaj et al. *J. Chem. Phys.* **147**, 191101–191102 (2017)

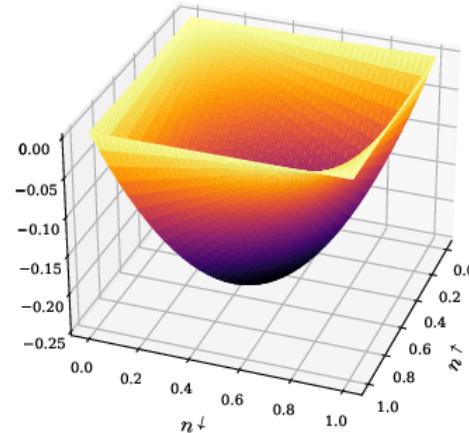
... but the $+J$ functional is not the right shape!



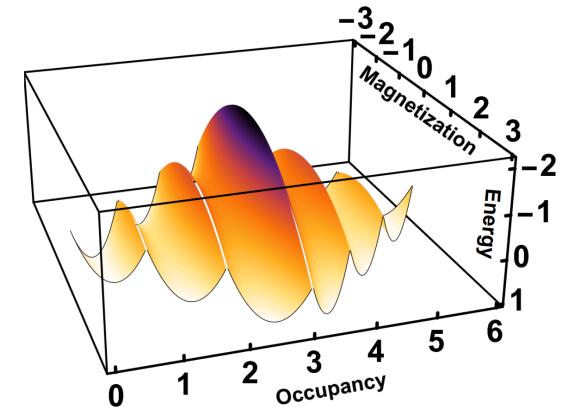
This served as inspiration for the BLOR functional³



correction to SIE

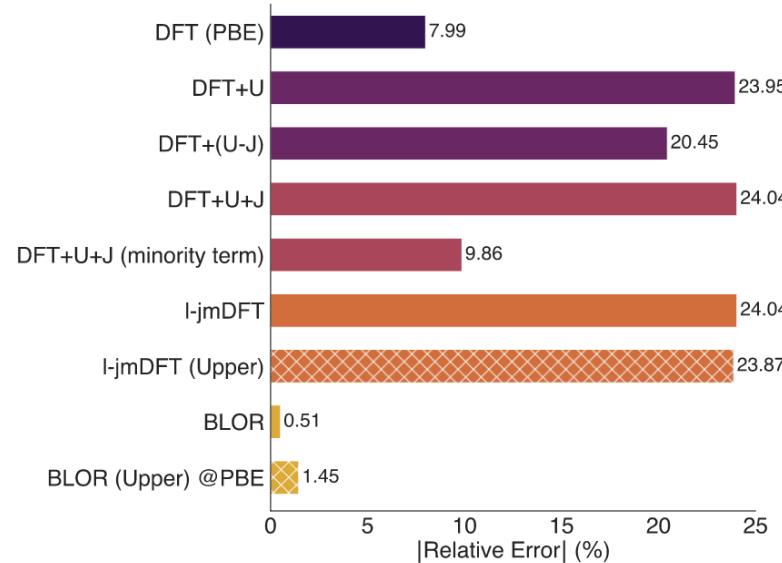


correction to SCE

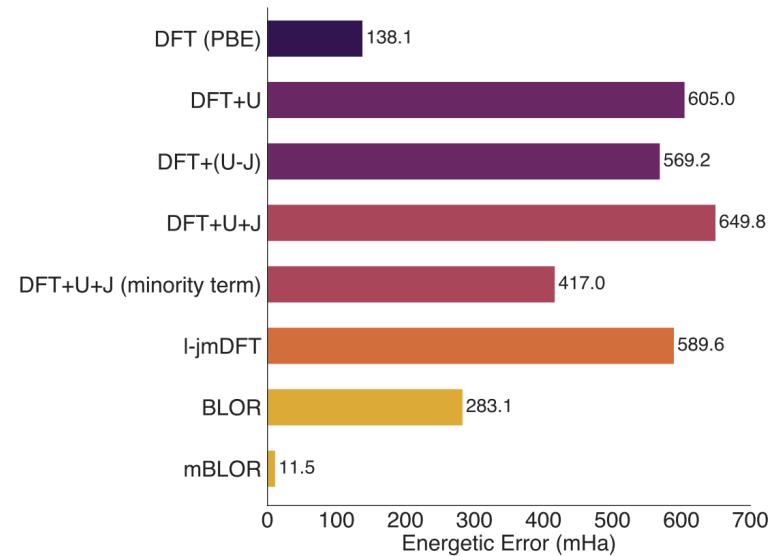


correction to both for a multi-projector subspace

³A. C. Burgess *et al.* *Phys. Rev. B* **107**, L121115 (2023), A. C. Burgess *et al.* (2024) doi:10.48550/arXiv.2408.08391



non-spin-polarized stretched H_2



non-spin-polarized stretched O_2

Koopmans functionals

$$E_{\text{KI}}^{\boldsymbol{\alpha}}[\{\rho_i\}] = E_{\text{DFT}}[\rho] + \sum_i \alpha_i [-(E_{\text{Hxc}}[\rho] - E_{\text{Hxc}}[\rho - \rho_i]) + f_i(E_{\text{Hxc}}[\rho - \rho_i + n_i] - E_{\text{Hxc}}[\rho - \rho_i])]$$

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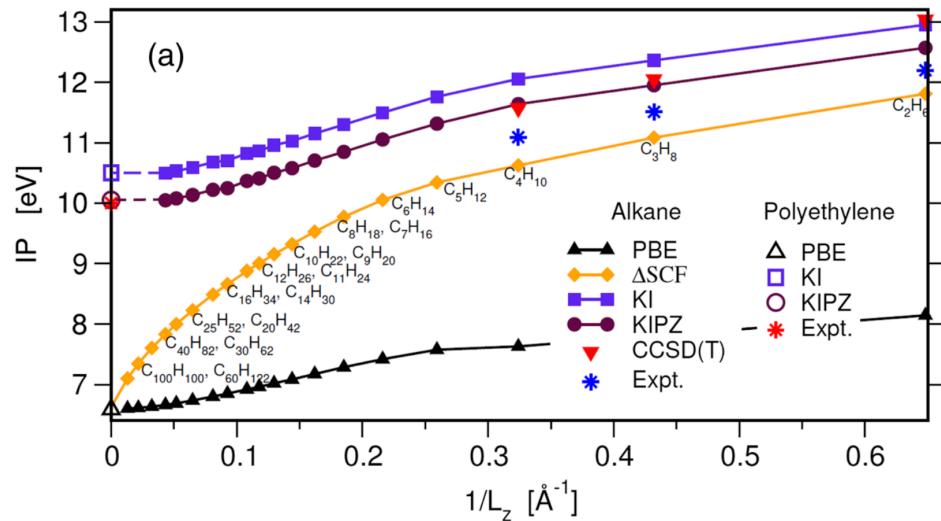
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- enforces $\frac{d^2 E}{df_i^2} = 0$, where $\{f_i\}$ is the occupation of some set of orbitals $\{\varphi_i\}$
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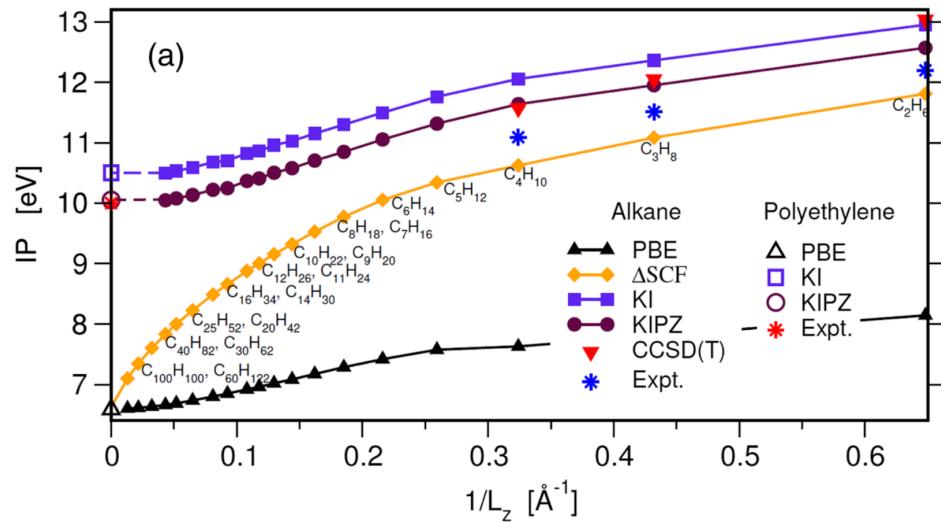
- enforces $\frac{d^2 E}{d f_i^2} = 0$, where $\{f_i\}$ is the occupation of some set of orbitals $\{\varphi_i\}$
- if $\{\varphi_i\}$ are eigenstates then this is GPWL

The problem with bulk systems



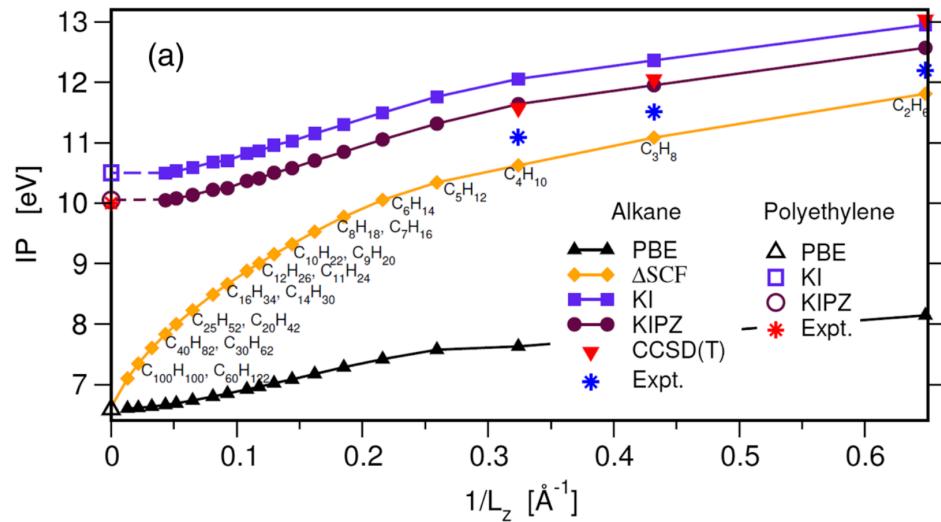
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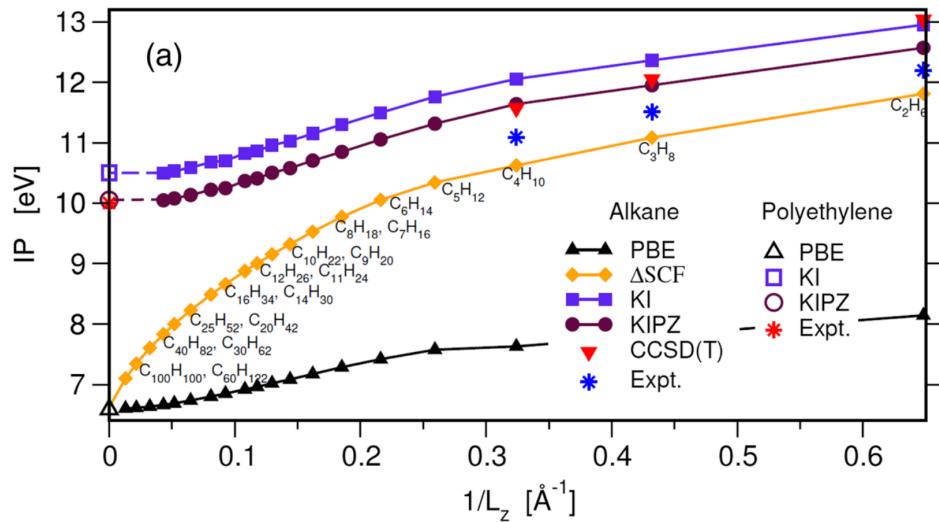


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But now we must ask

- why does correcting GPWL for Wannier functions work?
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The problem with bulk systems



- if applied to eigenstates the correction fails for bulk systems
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But now we must ask

- why does correcting GPWL for Wannier functions work?
- off-diagonal corrections?

A brief survey

method

DFT+*U*

DFT+*U+V*

DFT+*U+J*

imposes

$$\frac{d^2 E}{d(\lambda_i^{I\sigma})^2} = 0$$

$$\frac{d^2 E}{d(n^{IJ\sigma})d(n^{JI\sigma})} = 0?$$

$\frac{d^2 E}{d(m^I)^2} = 0?$ – but
wrong shape

with respect to the occupation of...

orbitals that diagonalize $n^{I\sigma}$; assumes a subsystem weakly interacting with the bath/frontier orbitals all lie within the subspace

orbitals that diagonalize $n^{I\sigma}$ mixed with projectors of adjacent sites

same as DFT+*U*

method	imposes	with respect to the occupation of...
BLOR	$\frac{d^2E}{dn^2} = 0;$ $\frac{d^2E}{dm^2} = 0$	projectors
mBLOR	$\frac{d^2E}{dN^2} = 0;$ $\frac{d^2E}{dM^2} = 0$	orbitals that diagonalize $n^{I\sigma}$
Koopmans (molecules)	$\frac{d^2E}{df_i^2} = 0 \quad \forall i$	KS eigenstates; fails in bulk limit

method

imposes

with respect to the occupation of...

Koopmans
(solids)

$$\frac{d^2 E}{df_i^2} = 0 \quad \forall i$$

Wannier functions; succeeds in bulk limit but subspace definition now arbitrary and we have a disconnect with GPWL

GSC¹

$$\frac{d^2 E}{df_i^2} = 0 \quad \forall i$$

KS eigenstates; equivalent to Koopmans for molecules

LOSC²

$$\frac{d^2 E}{df_i df_j} = 0 \quad \forall i, j$$

DLWFs (i.e. a set of localized orbitals)

¹Y. Mei *et al.* *J. Phys. Chem. Lett.* **12**, 7236–7244 (2021)

²A. Mahler *et al.* *Phys. Rev. B* **106**, 35147–35148 (2022)

Where to next?

I am **not** advocating for abandoning pragmatic corrections.

¹A. Tamai *et al.* *Phys. Rev. X* **9**, 21048–21049 (2019)

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Open questions:

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Open questions:

- what are the best criteria for choosing the orbitals/subspaces?

-

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Open questions:

- what are the best criteria for choosing the orbitals/subspaces? Do we need to turn to...
 - understanding the structure of self-energies¹?
 - ensemble DFT?
- are off-diagonal corrections to these orbitals/subspaces physical?
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- what are the best criteria for choosing the orbitals/subspaces? Do we need to turn to...
 - understanding the structure of self-energies¹?
 - ensemble DFT?
- are off-diagonal corrections to these orbitals/subspaces physical?
- are we expecting too much of our approximations?
 - e.g. BLOR and SCE – easier with reduced density matrix functional theory?

¹A. Tamai *et al.* *Phys. Rev. X* **9**, 21048–21049 (2019)

Thank you!

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