# The ATOMPAW generator


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- Brief history
- Validation
- Extensions


[a] Collaborators include Alan Tackett (Vanderbilt U.), Marc Torrent and François Jollet (CEA, France), and Xiao Xu (WFU). Yann Pouillon (UPV/EHU) implemented the build scripts. Work Supported by NSF grants DMR-0405456, 0427055, and 0705239; computations were performed on the Wake Forest University DEAC cluster.

# Brief History Leading to PAW

- Kleinman and Bylander, PRL **48** 1425 (1982) "*Efficacious Form for Model Pseudopotentials.*"
  Separable Form for Non-Local Pseudopotentials $\hat{\mathbf{V}}_{\mathbf{NL}} = \sum_{\mathbf{LM}} |\xi_{\mathbf{LM}}\rangle \delta \mathbf{V}_{\mathbf{L}} \langle \xi_{\mathbf{LM}}|$
- Gonze, Stumpf, and Scheffler, PRB **44** 8503 (1991) "*Analysis of Separable Potentials.*"
  Recipes for taming lurking "ghosts"
- Vanderbilt, PRB **41** 7892 (1990) "*Soft Self-Consistent Pseudopotentials in a Generalized Eigenvalue Formalism.*"
  Ultra-Soft Pseudopotentials (USPP)
- Blöchl, PRB **50** 17953 (1994) "*Projector augmented-wave method.*"
  PAW

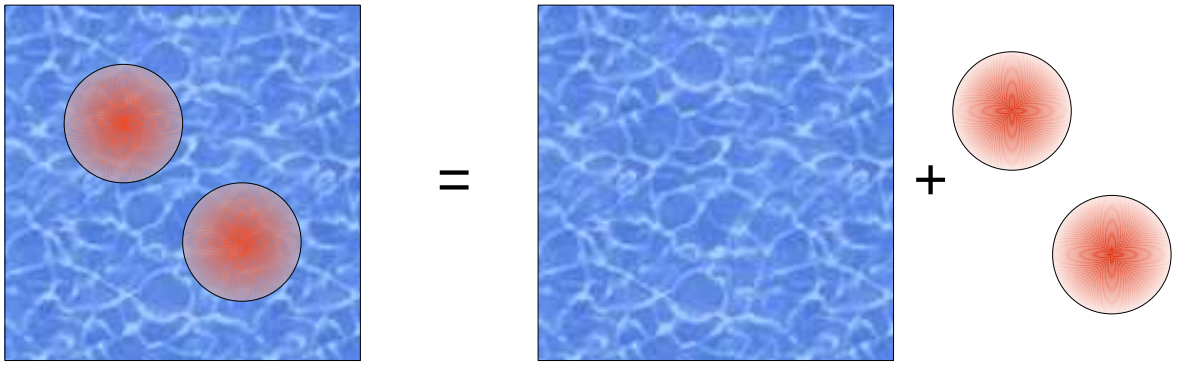
# The PAW Formalism

PAW transformation for a valence wavefunction:

$$\Psi_v(\mathbf{r}) = \widetilde{\Psi}_v(\mathbf{r}) + \sum_{ai} \left( \phi_i^a(\mathbf{r} - \mathbf{R}^a) - \widetilde{\phi}_i^a(\mathbf{r} - \mathbf{R}^a) \right) \langle p_i^a | \widetilde{\psi}_v \rangle. \qquad (1)$$

Partitioning of evaluation space. For example, the valence electron energy:

$$E_{tot}^{\text{vale}} = \underbrace{\widetilde{E}_{tot}}_{\text{pseudo energy}} + \sum_a \underbrace{\left( E_{tot}^a - \widetilde{E}_{tot}^a \right)}_{\text{atom-centered corrections}} . \qquad (2)$$



# Partitioning of the Coulomb Interactions

Both Hartree and Fock interactions can be expressed in terms of pair densities derived from products of two wavefunctions $\rho_{vw}(\mathbf{r}) \equiv \Psi_v^*(\mathbf{r})\Psi_w(\mathbf{r})$. The PAW transformation the these products take the form:

$$\rho_{vw}(\mathbf{r}) = \widetilde{\rho}_{vw}(\mathbf{r}) + \sum_a \left\{\rho^a_{vw}(\mathbf{r}-\mathbf{R}^a) - \widetilde{\rho}^a_{vw}(\mathbf{r}-\mathbf{R}^a)\right\}, \tag{3}$$

where

$$\widetilde{\rho}_{vw}(\mathbf{r}) \equiv \widetilde{\Psi}_v^*(\mathbf{r})\widetilde{\Psi}_w(\mathbf{r}), \tag{4}$$

and

$$\rho^a_{vw}(\mathbf{r}) - \widetilde{\rho}^a_{vw}(\mathbf{r}) \equiv \sum_{ij} \langle\widetilde{\Psi}_v|p^a_i\rangle\langle p^a_j|\widetilde{\Psi}_w\rangle \left\{\phi^{a*}_i(\mathbf{r})\phi^a_j(\mathbf{r}) - \widetilde{\phi}^{a*}_i(\mathbf{r})\widetilde{\phi}^a_j(\mathbf{r})\right\}. \tag{5}$$

Equivalently, we can write:

$$\rho_{vw}(\mathbf{r}) = \widetilde{\rho}_{vw}(\mathbf{r}) + \widehat{\rho}_{vw}(\mathbf{r}) + \sum_a \left(\rho^a_{vw}(\mathbf{r}-\mathbf{R}^a) - \widetilde{\rho}^a_{vw}(\mathbf{r}-\mathbf{R}^a) - \widehat{\rho}^a_{vw}(\mathbf{r}-\mathbf{R}^a)\right), \tag{6}$$

where the "compensation charge"

$$\widehat{\rho}_{vw}(\mathbf{r}) \equiv \sum_a \widehat{\rho}^a_{vw}(\mathbf{r}-\mathbf{R}^a) \tag{7}$$

is a smooth function localized within the atomic augmentation spheres such that:

$$\int d^3r' \, \frac{\rho^a_{vw}(\mathbf{r}') - \tilde{\rho}^a_{vw}(\mathbf{r}') - \hat{\rho}^a_{vw}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} = \begin{cases} V^a_{vw}(\mathbf{r}) & \text{for} \quad |\mathbf{r}-\mathbf{R}^a| \le r^a_c \\ 0 & \text{otherwise} \end{cases}. \tag{8}$$

# ATOMPAW is 10 years old!

Computer Physics Communications 135 (2001) 329–347

Computer Physics Communications

www.elsevier.nl/locate/cpc

## A Projector Augmented Wave (PAW) code for electronic structure calculations, Part I: *atompaw* for generating atom-centered functions

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$\Rightarrow \{\phi_i(r), \widetilde{\phi}_i(r), \widetilde{p}_i(r)\}$ and $V_{loc}(r)$

Generate input to *pwpaw*, *abinit*, *socorro*, *quantum-espresso*

# Database of PAW Atomicdata Files
# http://pwpaw.wfu.edu

## Periodic Table of the Elements for PAW Functions

| | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 H | | | | | | | | | | | | | | | | | 2 He |
| 3 Li | 4 Be | | | | | | | | | | | 5 B | 6 C | 7 N | 8 O | 9 F | 10 Ne |
| 11 Na | 12 Mg | | | | | | | | | | | 13 Al | 14 Si | 15 P | 16 S | 17 Cl | 18 Ar |
| 19 K | 20 Ca | 21 Sc | 22 Ti | 23 V | 24 Cr | 25 Mn | 26 Fe | 27 Co | 28 Ni | 29 Cu | 30 Zn | 31 Ga | 32 Ge | 33 As | 34 Se | 35 Br | 36 Kr |
| 37 Rb | 38 Sr | 39 Y | 40 Zr | 41 Nb | 42 Mo | 43 Tc | 44 Ru | 45 Rh | 46 Pd | 47 Ag | 48 Cd | 49 In | 50 Sn | 51 Sb | 52 Te | 53 I | 54 Xe |
| 55 Cs | 56 Ba | | 72 Hf | 73 Ta | 74 W | 75 Re | 76 Os | 77 Ir | 78 Pt | 79 Au | 80 Hg | 81 Tl | 82 Pb | 83 Bi | 84 Po | 85 At | 86 Rn |
| 87 Fr | 88 Ra | | 104 Rf | 105 Db | 106 Sg | 107 Bh | 108 Hs | 109 Mt | 110 Uun | 111 Uuu | 112 Uub | | 114 Uuq | | 116 Uuh | | |

| | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 57 La | 58 Ce | 59 Pr | 60 Nd | 61 Pm | 62 Sm | 63 Eu | 64 Gd | 65 Tb | 66 Dy | 67 Ho | 68 Er | 69 Tm | 70 Yb | 71 Lu | |
| | | 89 Ac | 90 Th | 91 Pa | 92 U | 93 Np | 94 Pu | 95 Am | 96 Cm | 97 Bk | 98 Cf | 99 Es | 100 Fm | 101 Md | 102 No | 103 Lr | |

Key

Modified Elements (using ≥atompaw_2.1) | Unmodified Elements (2005)

Comments

- The contents of this periodic table were created by John Tumbleston (currently a graduate student at UNC) and modified by Nick Dellaripa, David Harris, and Xiao Xu under the guidance of N.A.W. Holzwarth

# ATOMPAW User's Manual by Marc Torrent

## A user's guide for *atompaw* code

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*Commissariat à l'Energie Atomique et aux Energies Alternatives*
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Contact emails : marc.torrent@cea.fr, natalie@wfu.edu
Source code URL : http://pwpaw.wfu.edu

*Revised November 4th, 2010*

*Compatible with **atompaw v3.0** and later*

# Consistency of *abinit* and *pwpaw*

Computer Physics Communications 181 (2010) 1862–1867

Contents lists available at ScienceDirect

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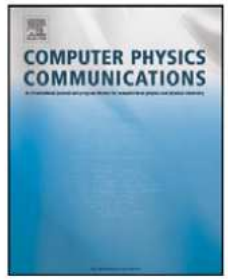


## Electronic structure packages: Two implementations of the projector augmented wave (PAW) formalism

Marc Torrent [a], N.A.W. Holzwarth [b,*], François Jollet [a], David Harris [b], Nicholas Lepley [b], Xiao Xu [b]

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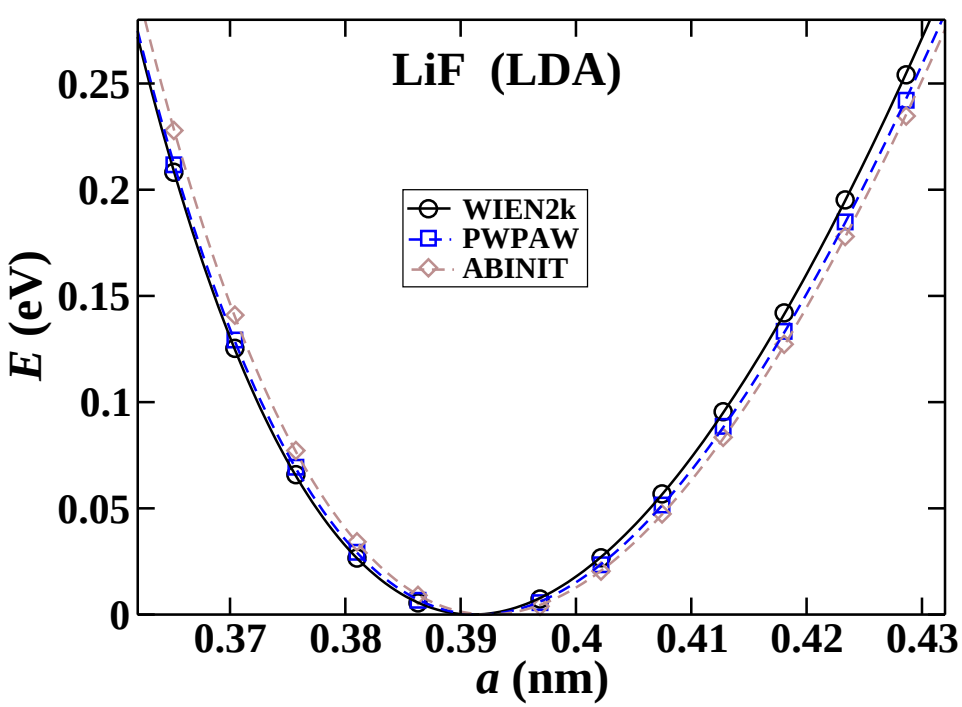
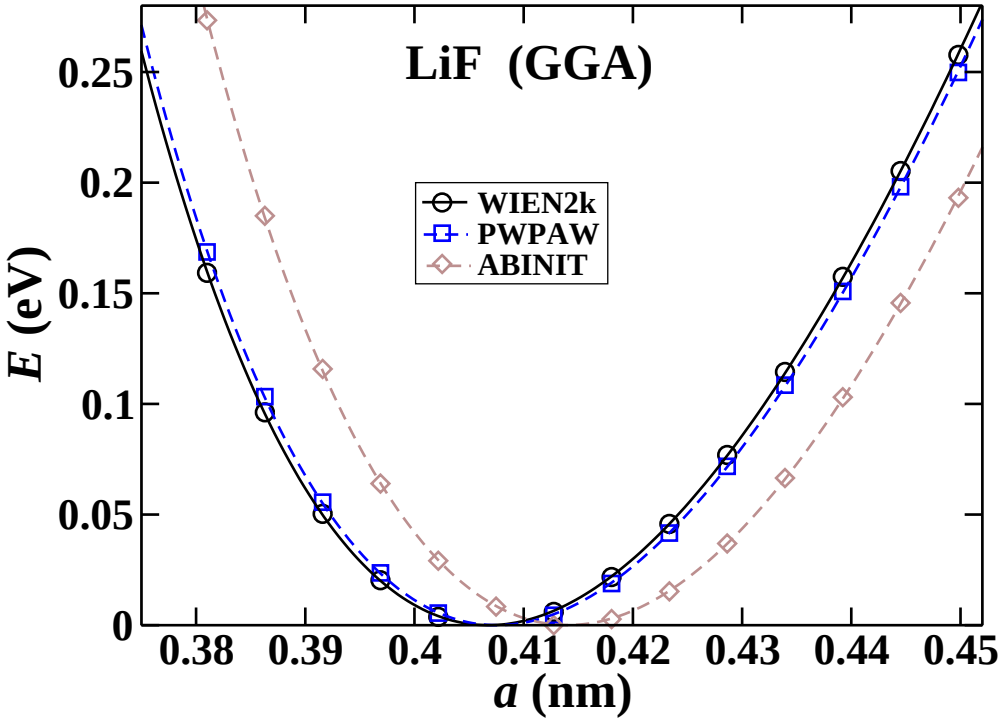
# Mystery < 2010




LDA binding energy curve for LiF




GGA binding energy curve for LiF

# Mystery Traced to Exchange-Correlation Terms

## Blöchl's formulation

(PRB **50**, 17953 (1994))

$$E_{xc}^{\mathrm{B}} = E_{xc}[\widetilde{n} + \widetilde{n}_c] + \sum_a \left( E_{xc}^a[n^a + n_c^a] - E_{xc}^a[\widetilde{n}^a + \widetilde{n}_c^a] \right).$$

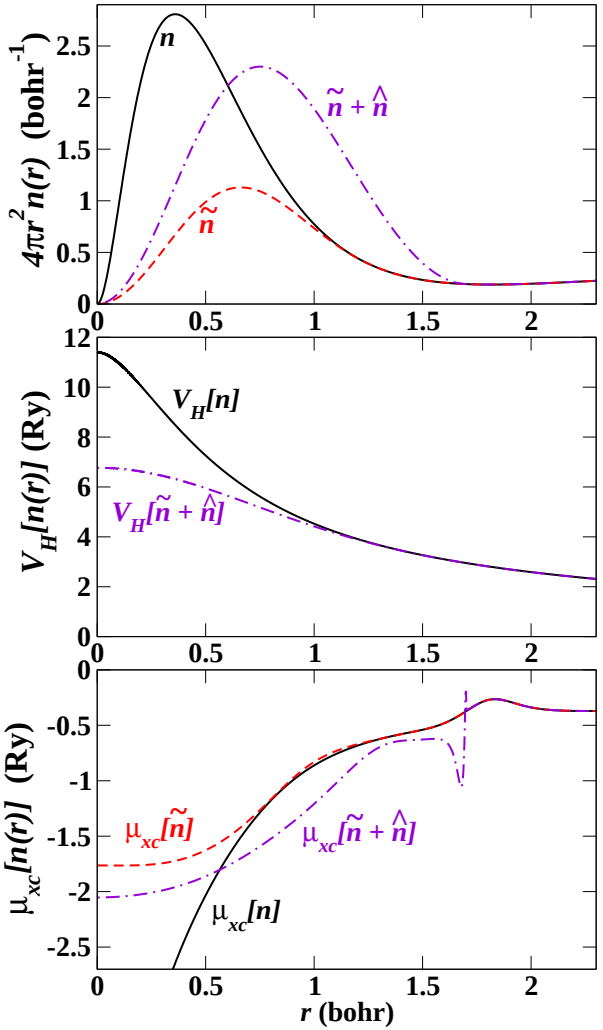
## Kresse's formulation

(PRB **59**, 1758 (1999))

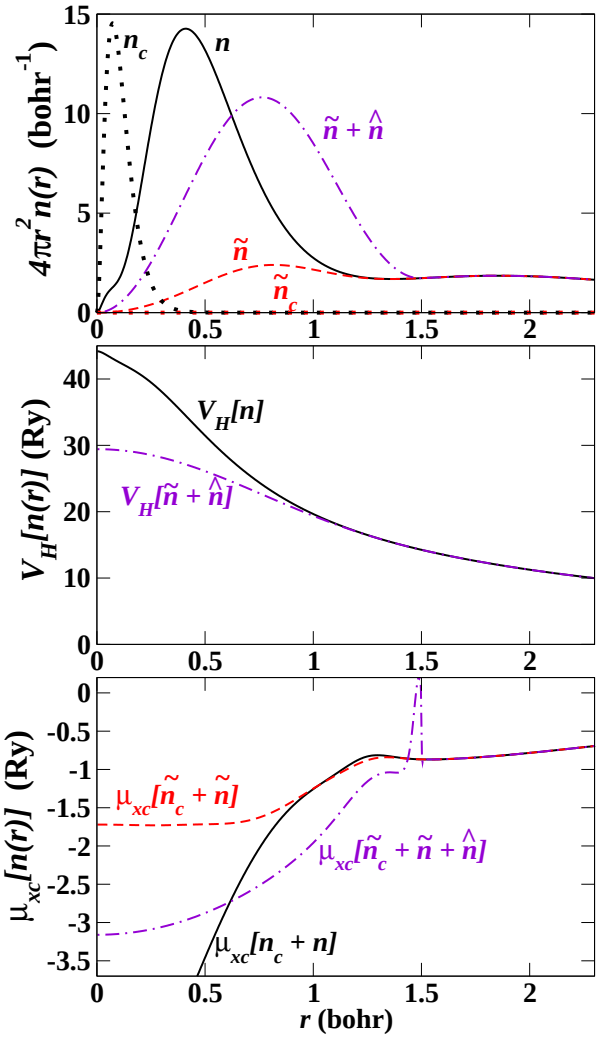
$$E_{xc}^{\mathrm{K}} = E_{xc}[\widetilde{n} + \widetilde{n}_c + \hat{n}] + \sum_a \left( E_{xc}^a[n^a + n_c^a] - E_{xc}^a[\widetilde{n}^a + \widetilde{n}_c^a + \hat{n}^a] \right).$$

# Example Exchange-Correlation Potentials

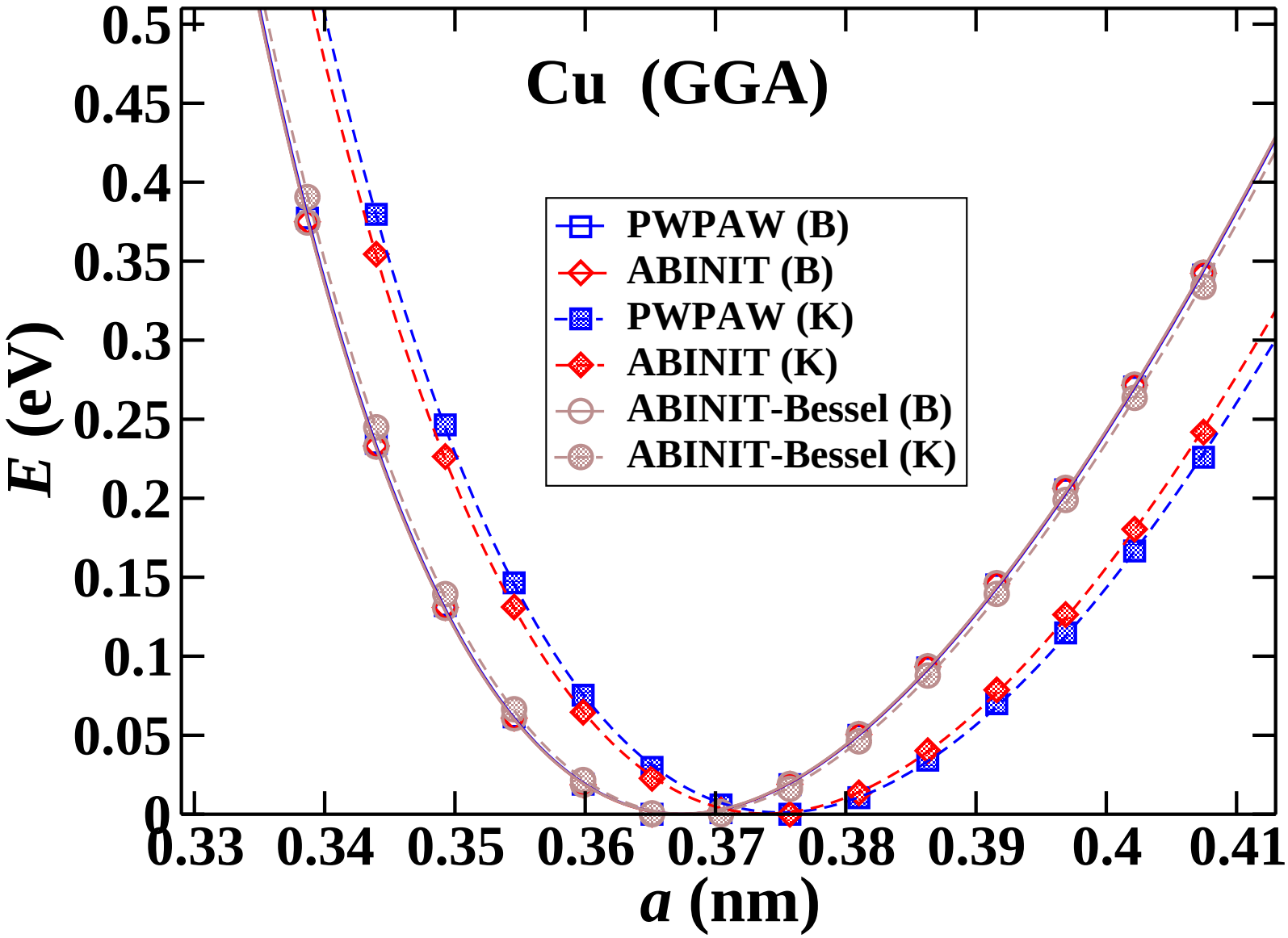
**Li GGA** $(1s^2 2s^1)$




**Si GGA** $(2s^2 3s^2 2p^6 3p^2)$

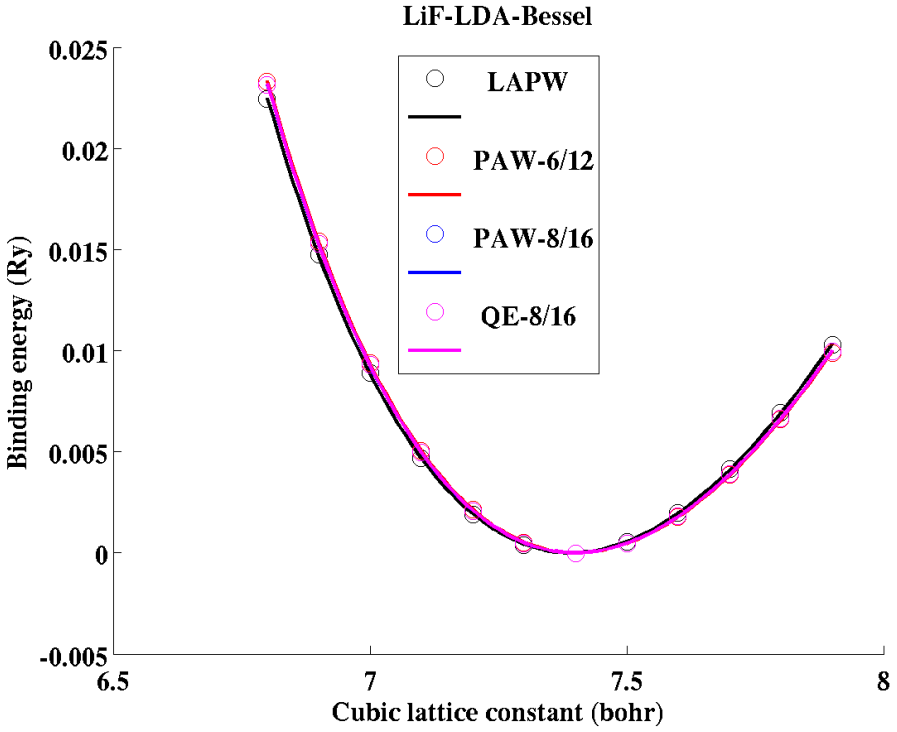


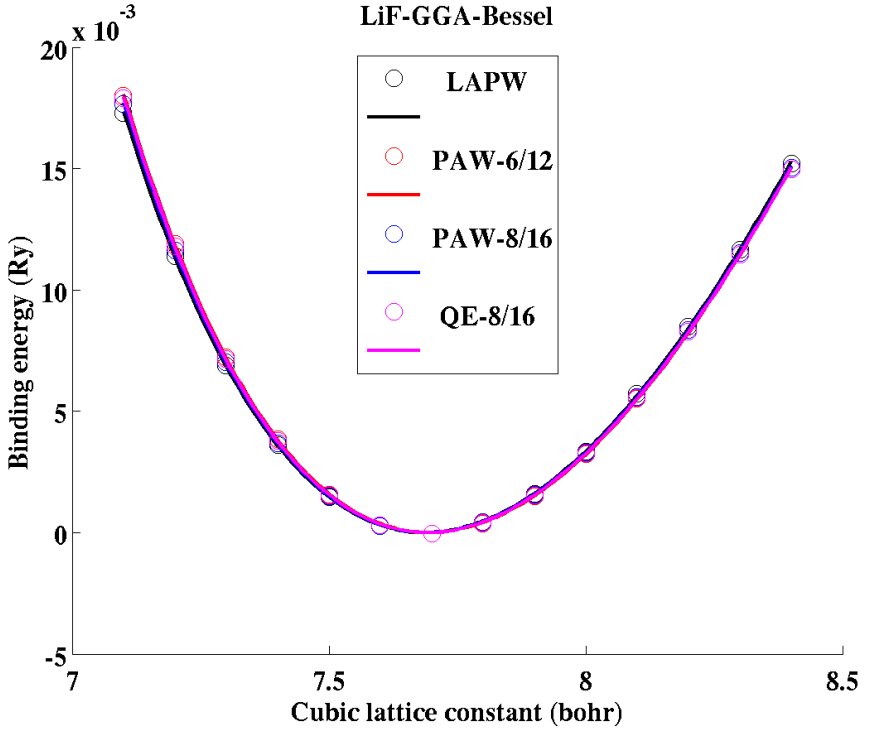
# Mystery Solved – *abinit* and *pwpaw* now agree




Bind energy curves for fcc Cu using GGA, comparing Blöchl and Kresse formulations.

# Validation: Consistency between various codes



Heats of formation $\Delta H_{\mathrm{cal}}$ (eV per formula unit) calculated for the lithium (thio)phosphate and related materials, comparing USPP, PAW and experiment (CRC or NIST).

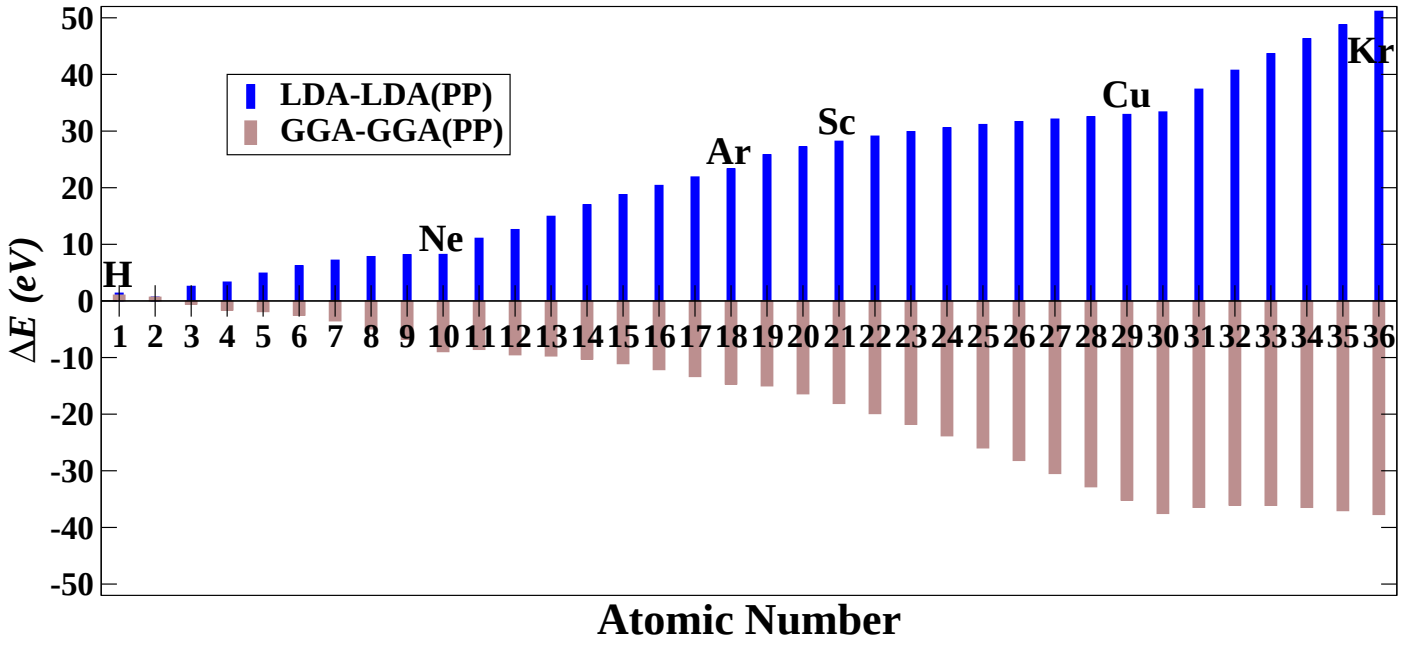
| Material | (USPP) | (PAW) | exp |
|---|---|---|---|
| $Li_2O$ | -6.18 | -6.19 | -6.20 |
| $Li_2O_2$ | -6.53 | -6.52 | -6.57 |
| $\beta$-$Li_3PO_4$ | -21.41 | -21.39 | |
| $\gamma$-$Li_3PO_4$ | -21.38 | -21.36 | -21.72 |
| $Li_4P_2O_6$ | -30.02 | -29.93 | |
| $Li_4P_2O_7$ | -34.25 | -34.21 | |
| $Li_7P_3O_{11}$ | -55.26 | -55.26 | |
| $Li_2S$ | -4.30 | -4.30 | -4.57 |
| $Li_2S_2$ | -4.10 | -4.10 | |
| $\beta$-$Li_3PS_4$ | -8.39 | -8.35 | |
| $\gamma$-$Li_3PS_4$ | -8.19 | -8.16 | |
| $Li_4P_2S_6$ | -12.45 | -12.38 | |
| $Li_4P_2S_7$ | -11.62 | -11.54 | |
| $Li_7P_3S_{11}$ | -20.06 | -19.94 | |
| $SO_3$ | -4.83 | -4.86 | -4.71 |
| $Li_2SO_4$ | -14.74 | -14.76 | -14.89 |

## Ongoing work – extension of PAW formalism to orbital dependent functionals

- Motivation
- Treatment of core electrons
- Hartree-Fock equations
- Approximate OEP equations (KLI)

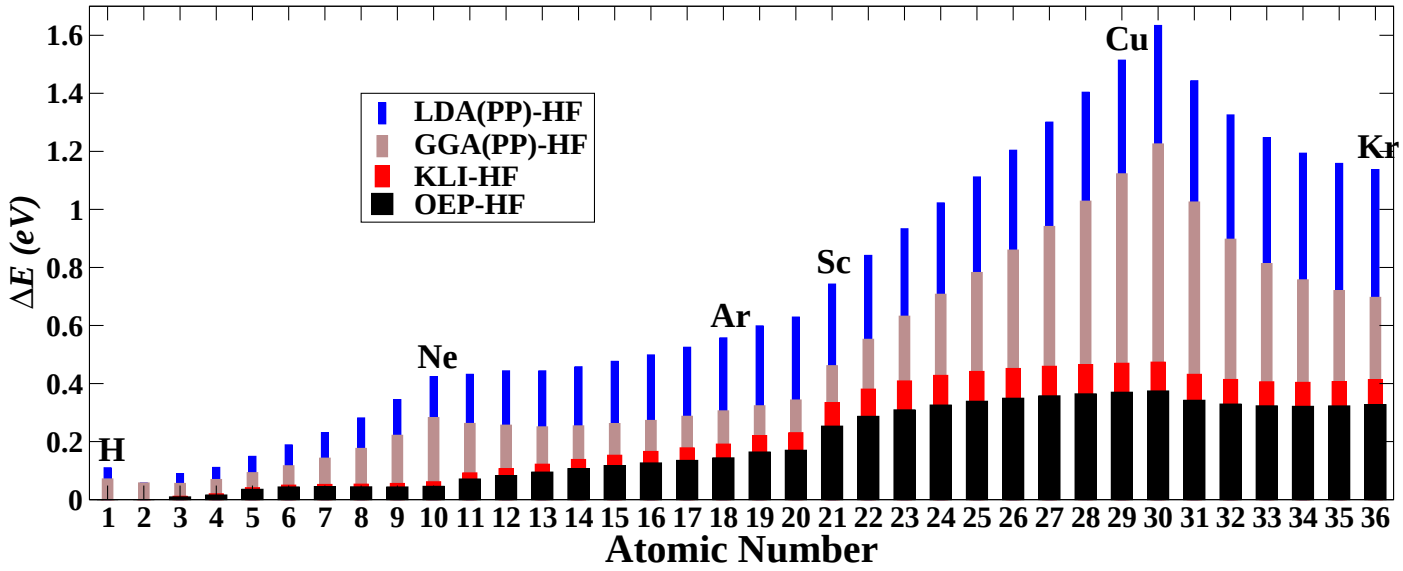
# "Post-processing" estimate of Fock exchange relative to self-consistent LDA or GGA Results

$$E_{xc}^{\mathrm{GGA/LDA}} - E_{x}^{\mathrm{Fock}}$$



# Comparison of Self-Consistent and "post-processing" Treatments of Fock exchange

$$E_{tot}^{OEP/KLI/PP} - E_{tot}^{HF}$$




"KLI" reference: Krieger, Li, and Iafrate, PRA **45**, 101 (1992)

More recent perspective on OEP and KLI: Bulat and Levy, PRB **80**, 052510 (2009)

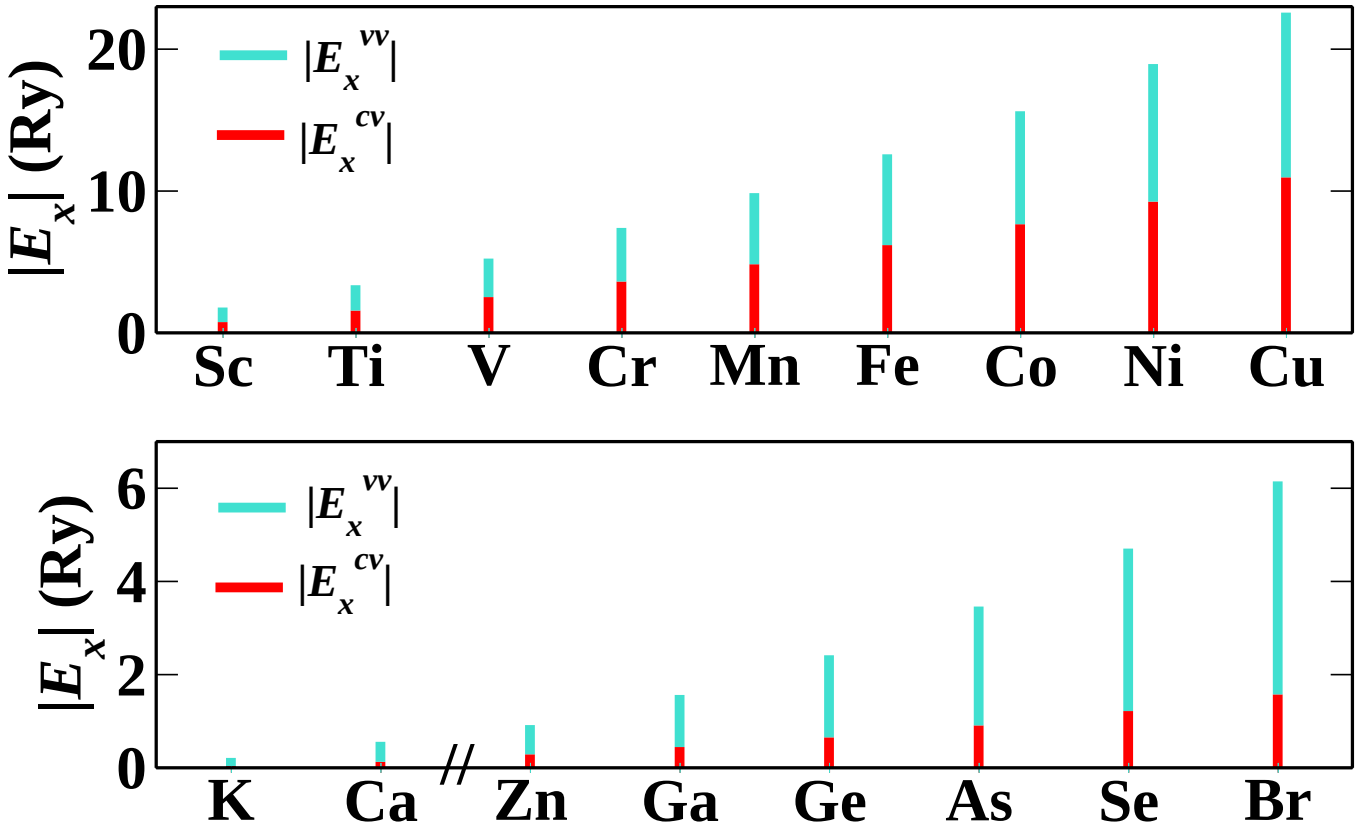
# Orbital Dependent Functionals

## Fock Exchange Energy

$$E_x \equiv -e^2 \sum_{pq}{}' \int\int d^3r d^3r' \frac{\Psi_p^*(\mathbf{r})\Psi_q(\mathbf{r})\Psi_q^*(\mathbf{r}')\Psi_p(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

## Core and Valence Electron Contributions to Fock Exchange Energy

$$E_x \equiv E_x^{vv} + E_x^{cv} + E_x^{cc}$$



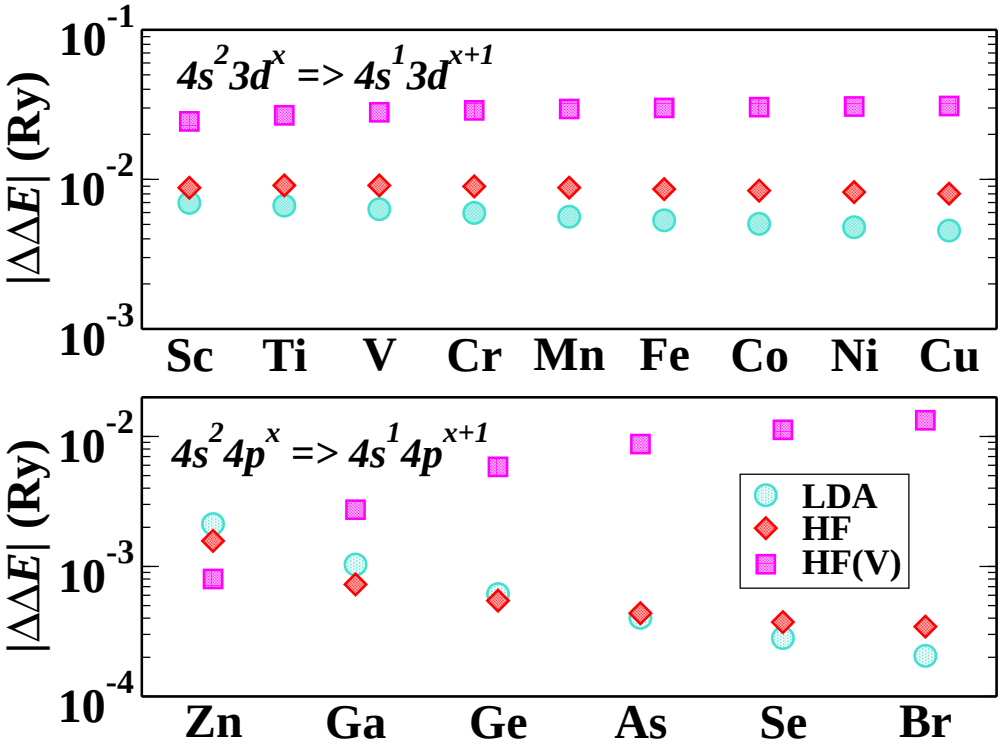
# Core-Valence contributions in Fock Exchange

√ **Frozen Core *Orbital* Approximation to Fock Exchange Energy**

$$E_x^{cv} \approx -e^2 \sum_{vc} \int\int d^3r d^3r' \frac{\Psi_v^*(\mathbf{r})\bar{\Psi}_c(\mathbf{r})\bar{\Psi}_c^*(\mathbf{r}')\Psi_v(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

**Frozen Core *Potential* Approximation to Fock Exchange Energy**

$$E_x^{cv} \approx \int d^3r V_x^{cv}(\mathbf{r})\rho_v(\mathbf{r})$$




Frozen core *orbital* and frozen core *potential* errors in various excitation energies.

# Hartree Fock Equations for Atoms

Xu and Holzwarth, PRB **81**, 245105 (2010)

$$H^{\rm HF}(r)\psi_p^{\rm HF}(r) + X_p(r) - \sum_{q;N_q>0} \lambda_{qp}\psi_q^{\rm HF}(r) = 0.$$

Here,

$$H^{\rm HF}(r) \equiv \mathcal{K} + V_N(r) + V_H(r). \tag{9}$$

The exchange kernel function is given by

$$X_p(r) \equiv \frac{1}{N_p}\frac{\delta E_x}{\delta \psi_p^*} = -\sum_q \sum_{L=|l_p-l_q|}^{l_p+l_q} \frac{1}{N_p}\Theta_{pq}^L\, W_{qp}^L(r)\psi_q^{\rm HF}(r),$$

where

$$W_{qp}^L(r) \equiv e^2 \int dr'\, \frac{r_<^L}{r_>^{L+1}}\psi_q^{\rm HF*}(r')\psi_p^{\rm HF}(r').$$

# Hartree Fock PAW Equations for Atoms

$$\mathcal{H}_{\rm HF}^{\rm PAW}(\mathbf{r})\widetilde{\Psi}_v^{\rm HF}(r) + X_v^{\rm PAW}(\mathbf{r}) - \sum_q \lambda_{qv}\mathcal{O}_{\rm HF}^{\rm PAW}\widetilde{\Psi}_q^{\rm HF}(\mathbf{r}) = 0.$$

The single particle term takes the form

$$\mathcal{H}_{\rm HF}^{\rm PAW}(\mathbf{r}) = \widetilde{\mathcal{H}}^{\rm HF} + \sum_{aij} |\widetilde{P}_i^a\rangle D_{ij}^{a\rm HF}\langle\widetilde{P}_j^a|,$$

where the pseudo Hamiltonian-like terms depend on the pseudopotentials due to the nuclear and Hartree interactions:

$$\widetilde{\mathcal{H}}^{\rm HF}(\mathbf{r}) \equiv \mathcal{K} + \widetilde{V}_N(\mathbf{r}) + \widetilde{V}_H(\mathbf{r}). \tag{10}$$

The exchange function term takes the form

$$X_v^{\rm PAW}(\mathbf{r}) = \widetilde{X}_v(\mathbf{r}) + \sum_{ai} |\widetilde{P}_i^a\rangle X_{iv}^a,$$

where the pseudo-exchange kernel function takes the form:

$$\widetilde{X}_v(r) \equiv -\sum_q \sum_{L=|l_v-l_q|}^{l_v+l_q} \frac{1}{N_v}\Theta_{vq}^L\ \widetilde{W}_{qv}^L(r)\widetilde{\psi}_q^{\rm HF}(r).$$

$$\widetilde{W}_{qv}^L(r) \equiv e^2 \int dr'\ \frac{r_<^L}{r_>^{L+1}}\left(\widetilde{\psi}_q^{\rm HF*}(r')\widetilde{\psi}_v^{\rm HF}(r') + M_{qv}^L(r')\right).$$

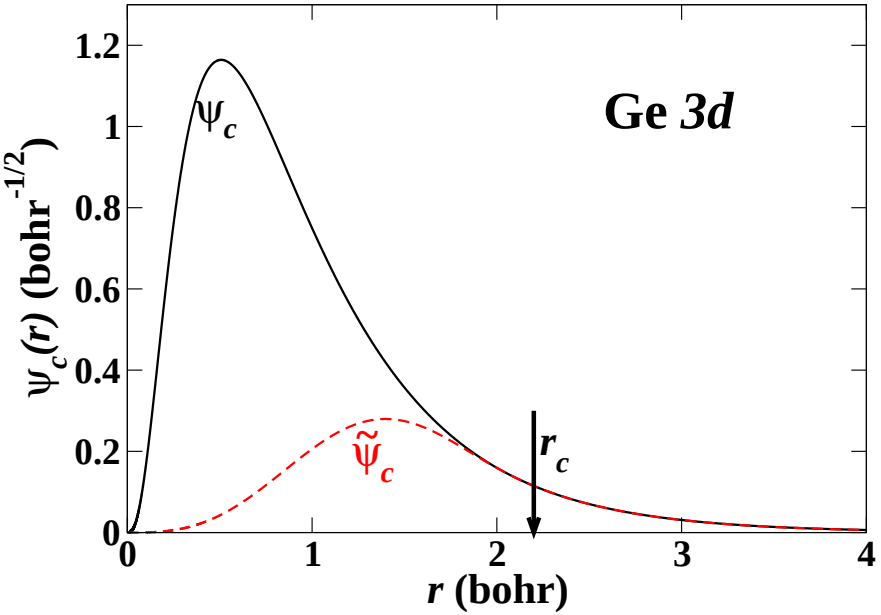
# Hartree Fock PAW Equations for Atoms – (continued)

$$
\begin{aligned}
X^a_{iv} = & -\sum_{v'} \sum_{L=|l_v - l_{v'}|}^{l_v + l_{v'}} \frac{1}{N_v} \Theta^L_{vv'} \\
& \times \left( \sum_{jkl} \langle \widetilde{P}^a_j | \widetilde{\Psi}^{\mathrm{HF}}_{v'} \rangle \langle \widetilde{\Psi}^{\mathrm{HF}}_{v'} | \widetilde{P}^a_k \rangle \langle \widetilde{P}^a_l | \widetilde{\Psi}^{\mathrm{HF}}_{v} \rangle \left( R^{aL}_{ij;kl} - \widetilde{R}^{aL}_{ij;kl} \right) \right. \\
& \left. + \sum_j \langle \widetilde{P}^a_j | \widetilde{\Psi}^{\mathrm{HF}}_{v'} \rangle Z^{aL}_{v'v;ij} \right) \\
& - \sum_{c} \sum_{L=|l_v - l_c|}^{l_v + l_c} \frac{1}{N_v} \Theta^L_{vc} \left( \sum_j \langle \widetilde{P}^a_j | \widetilde{\Psi}^{\mathrm{HF}}_{v} \rangle \left( R^{aL}_{ic;cj} - \widetilde{R}^{aL}_{ic;cj} \right) \right. \\
& \left. + Z^{aL}_{cv;ic} \right),
\end{aligned}
$$

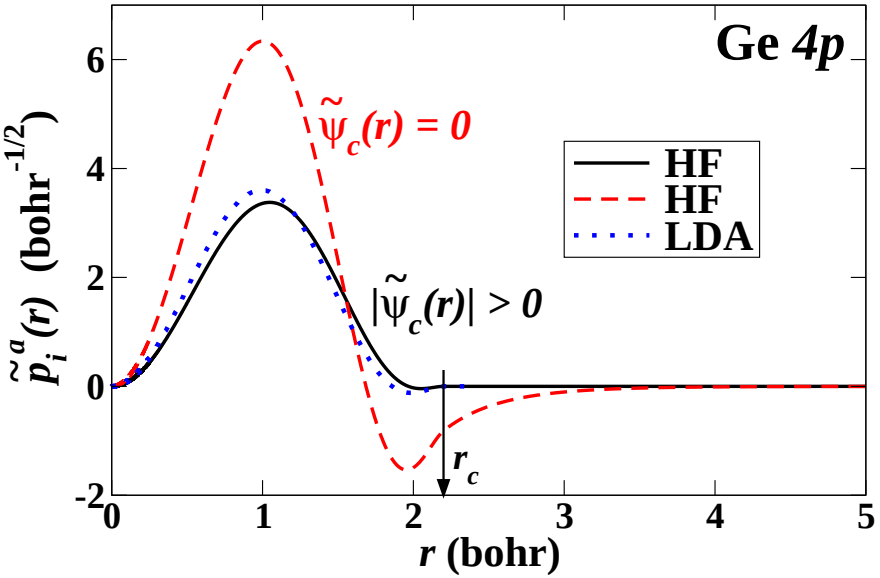
where

$$
Z^{aL}_{qv;ij} \equiv \int dr \widetilde{W}^L_{qv}(r) \widehat{m}^{aL}_{ij}(r). \tag{11}
$$

# Some details about "extended" core states




Radial Hartree-Fock wavefunction $\psi_c(r)$ for the $3d$ core state of Ge compared with the constructed pseudo-wavefunction $\widetilde{\psi}_c(r)$.




Radial PAW projector functions for $4p$ states of Ge, comparing effects of including and excluding pseudo-core orbital functions $\widetilde{\psi}_c(r)$ within the Hartree-Fock (HF) formulation and also comparing the corresponding LDA projector.

# Some details about Kohn-Sham *vs* Hartree-Fock projector functions

## Kohn-Sham

$$\left(\widetilde{\mathcal{H}}^{\rm KS}(r) - \varepsilon_i^a\right) \widetilde{\Phi}_i^a(\mathbf{r}) = \sum_j \widetilde{P}_j^a(\mathbf{r}) \langle \widetilde{\Phi}_j^a | \widetilde{\mathcal{H}}^{\rm KS} - \varepsilon_i^a | \widetilde{\Phi}_i^a \rangle$$

## Hartree-Fock

$$\widetilde{H}^{\rm HF}(\mathbf{r}) \widetilde{\Phi}_i^a(\mathbf{r}) + \widetilde{X}_i(\mathbf{r}) - \sum_{q;N_q>0} \lambda_{qi} \widetilde{\Psi}_q^{\rm HF}(\mathbf{r}) =$$

$$\sum_j \widetilde{P}_j^a(\mathbf{r}) \left( \langle \widetilde{\Phi}_j^a | \widetilde{H}^{\rm HF} | \widetilde{\Phi}_i^a \rangle + \langle \widetilde{\Phi}_j^a | \widetilde{X}_i \rangle - \sum_{q;N_q>0} \lambda_{qi} \langle \widetilde{\Phi}_j^a | \widetilde{\Psi}_q^{\rm HF} \rangle \right),$$

# Orbital Dependent Functionals + Kohn-Sham = Optimized Effective Potential (OEP) Formalism

## Fock Exchange Energy

$$E_x \equiv -e^2 \sum_{pq}{}' \int\int d^3r d^3r' \frac{\Psi_p^*(\mathbf{r})\Psi_q(\mathbf{r})\Psi_q^*(\mathbf{r}')\Psi_p(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

## Kohn-Sham Equations

$$H^{KS}(\mathbf{r})\Psi_p(\mathbf{r}) = \varepsilon_p \Psi_p(\mathbf{r})$$

$$H^{KS}(\mathbf{r}) \equiv \mathcal{K} + V_N(\mathbf{r}) + V_H(\mathbf{r}) + V_x(\mathbf{r})$$

$$V_x(\mathbf{r}) = \frac{\delta E_x}{\delta \rho(\mathbf{r})}$$

# KLI* approximation to Optimized Effective Potential (OEP) Formalism

* Krieger, Li, and Iafrate, PRA **45**, 101 (1992)

$$V_x^{\rm KLI}(r)\, n(r) = \sum_p N_p \psi_p(r) X_p^{\rm KLI}(r) + \sum_p N_p \left|\psi_p(r)\right|^2 \left(\bar{V}_{x\,p}^{\rm KLI} - \bar{U}_{x\,p}^{\rm KLI}\right)$$

where

$$n(r) \equiv \sum_p N_p \left|\psi_p(r)\right|^2$$

$$\sum_{q\neq o} \left[\delta_{pq} - \Gamma_{pq} N_q\right] \bar{V}_{x\,q}^{\rm KLI} = \Xi_p - \sum_{q\neq o} \Gamma_{pq} N_q \bar{U}_{x\,q}^{\rm KLI}.$$

Here

$$\Gamma_{pq} \equiv \int dr\, \frac{\left|\psi_p(r)\right|^2 \left|\psi_q(r)\right|^2}{n(r)},$$

and

$$\Xi_p \equiv \int dr\, \frac{\left|\psi_p(r)\right|^2 \sum_q N_q \psi_q(r) X_q^{\rm KLI}(r)}{n(r)}.$$

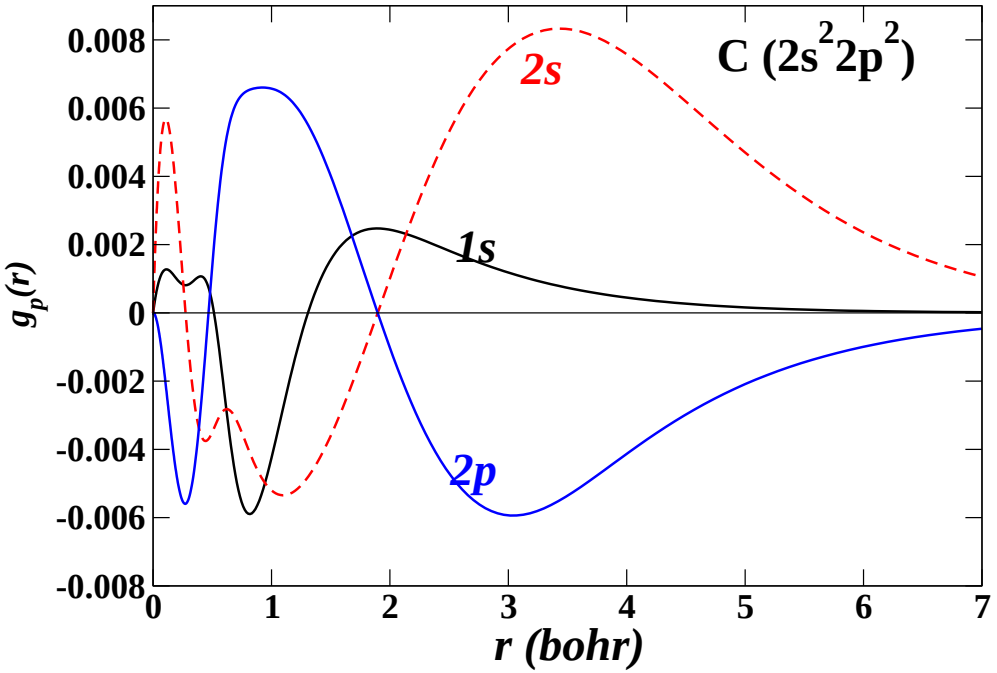
# Relationship between KLI approximation to OEP

Bulat and Levy, PRB **80**, 052510 (2009)

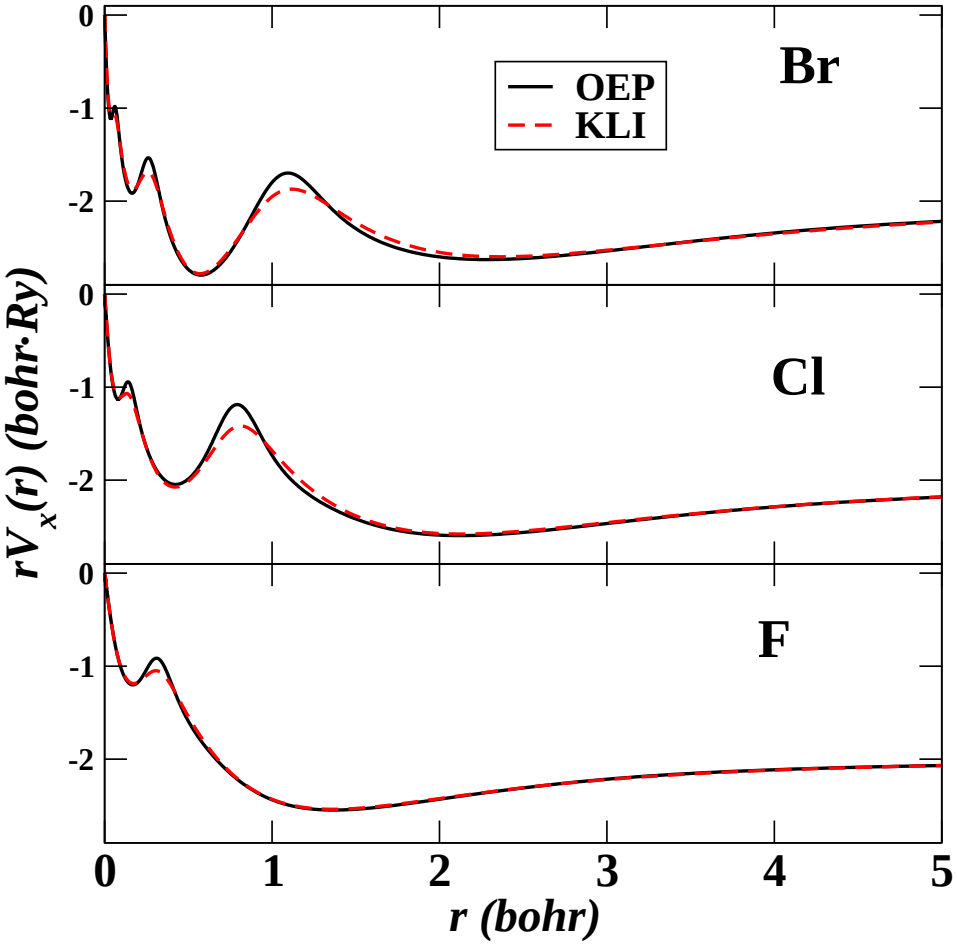
$$V_x^{\mathrm{OEP}}(r) = \underbrace{V_x^{occ}(r)}_{\text{slight extension to KLI}} + f(\{\phi_q^{unocc}(r)\}).$$

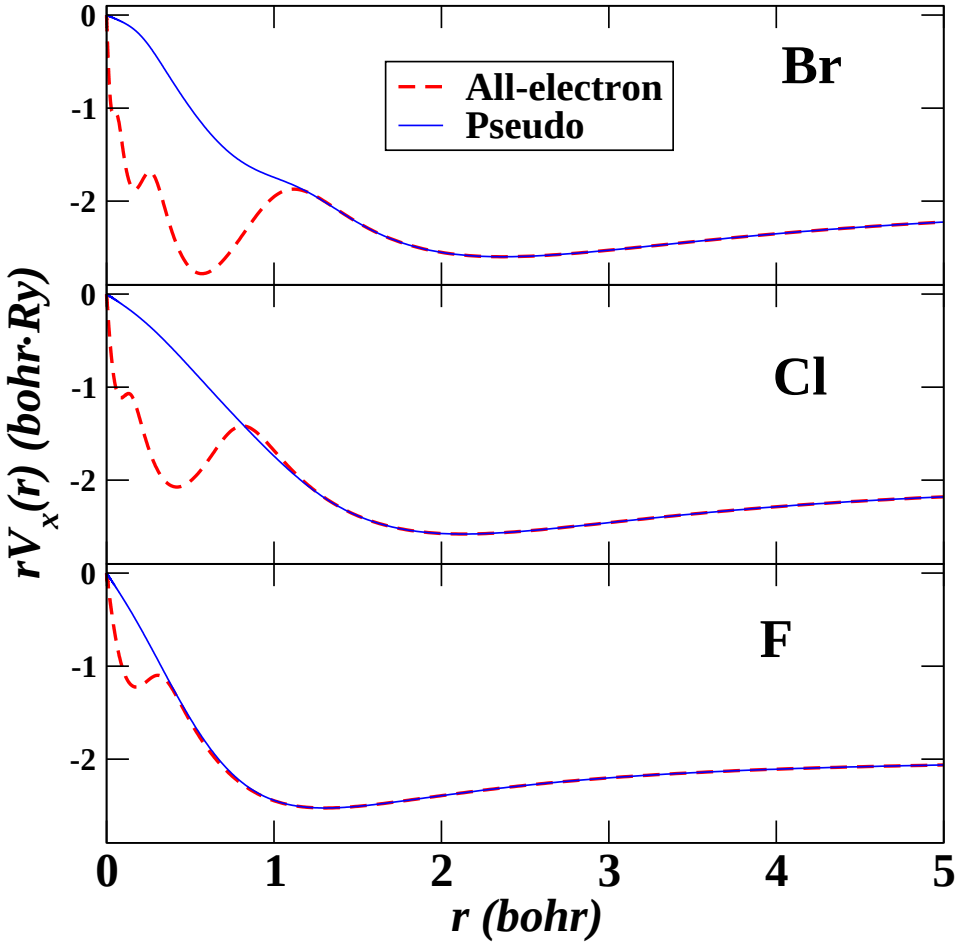
Orbital shift function of full OEP

$$(\mathcal{H} - \epsilon_p)\, g_p(r) = X_p(r) - V_x(r)\psi_p(r) - \left(\bar{U}_{x\ p} - \bar{V}_{x\ p}\right)\psi_p(r); \quad \sum_p N_p g_p(r)\psi_p(r) = 0.$$



# Comparison of $V_x(r)$ AE-OEP, AE-KLI, and PAW-KLI



# PAW-KLI formalism

$$V_x^{\rm KLI}(r)\, n(r) \Rightarrow \widetilde{V}_x^{\rm KLI}(r)\, \widetilde{n}(r) + \left( V_x^{a\rm KLI}(r)\, n^a(r) - \widetilde{V}_x^{a\rm KLI}(r)\, \widetilde{n}^a(r) \right).$$

$\Rightarrow$ Assume that each term satisfies the KLI equations in their respective spacial and functional domains.

$$\widetilde{V}_x^{\rm KLI}(r)\, \widetilde{n}(r) = \sum_v N_v \widetilde{\psi}_v(r) \widetilde{X}_v^{\rm KLI}(r) + \sum_v N_v \left| \widetilde{\psi}_v(r) \right|^2 \left( \bar{V}_{x\,v}^{\rm KLI} - \bar{U}_{x\,v}^{\rm KLI} \right).$$

$$V_x^{a\rm KLI}(r)\, n^a(r) = \sum_p N_p \psi_p^a(r) X_p^{a\rm KLI}(r) + \sum_p N_p \left| \psi_p^a(r) \right|^2 \left( \bar{V}_{x\,p}^{\rm KLI} - \bar{U}_{x\,p}^{\rm KLI} \right),$$

$$\widetilde{V}_x^{a\rm KLI}(r)\, \widetilde{n}^a(r) = \sum_v N_v \widetilde{\psi}_v^a(r) \widetilde{X}_v^{a\rm KLI}(r) + \sum_v N_v \left| \widetilde{\psi}_v^a(r) \right|^2 \left( \bar{V}_{x\,v}^{\rm KLI} - \bar{U}_{x\,v}^{\rm KLI} \right).$$

# Summary and Conclusions

- Thanks to the *abinit* community for continuously providing excellent computational tools, productive framework for collaboration, . . .
- *atompaw* now produces atomic datasets for *abinit*, *quantum espresso*, *pwpaw*, *socorro*
- For Fock exchange, we argue that the frozen core *orbital* approach offers better accuracy and is compatible with the PAW formalism.
- We have formulated the PAW equations for Hartree-Fock and KLI and are currently testing them in *pwpaw*.
- Future work –
  - Finish testing Hartree-Fock and KLI in *pwpaw*.
  - Extend approach to hybrid functionals ??
  - Possibly extend Hartree-Fock and KLI in other codes.