DFT: Exchange-Correlation

Local functionals, exact exchange and other post-DFT methods

Paul Tulip
Centre for Materials Physics
Department of Physics
University of Durham
Outline

• Introduction

• What is exchange and correlation?

• Quick tour of XC functionals
  – (Semi-)local: LDA, PBE, PW91, WC, etc
  – Ab initio non-local: HF, sX, OEP
  – Empirical non-local (hybrids): B3LYP, HSE
  – DFT+U
  – DFT+D
  – Beyond DFT: GW

• Appropriate Use

• Closing statements
Density Functional Theory

• Foundation is Hohenberg-Kohn-Sham approach

\[ n(r) \]

\[ n(r) \]

- Auxiliary system has **same** electronic density as N-electron system

- Auxiliary system particles are **non-interacting**

\[ \Rightarrow \quad \text{Kohn-Sham equations} \]

\[ \left( -\frac{\hbar^2}{2m} \nabla^2 + v_{\text{ext}}(r) + v_{\text{Hartree}}(r) + v_{\text{xc}}(r) \right) \phi_i(r) = \epsilon_i \phi_i(r) \]

\[ n(r) = \sum_i \phi_i^*(r) \phi_i(r) \]
Density Functional Theory

• Hohenberg-Kohn-Sham approach turns an intractable N-body problem into N coupled one-body problems

• This is tractable!

• QM exchange-correlation effects in $v_{xc}(r)$

• This is the great unknown in DFT – we must approximate

• Commonly used approximations: LDA, GGA, BLYP, B3LYP …. 
A Formal Definition

We can formally define the XC energy through:

\[
E_{xc}[n(\vec{r})] = T[n(\vec{r})] - T_s[n(\vec{r})] + E_{ee}[n(\vec{r})] - E_H[n(\vec{r})]
\]
A Formal Definition

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*cx* kinetic energy
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**Exact** kinetic energy

KS kinetic energy
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**Exact** kinetic energy

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**Exact** e-e interaction
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- **Exact** kinetic energy
- KS kinetic energy
- Hartree energy
- **Exact** e-e interaction
We can formally define the XC energy through:

\[ E_{xc}[n(\vec{r})] = T[n(\vec{r})] - T_s[n(\vec{r})] + E_{ee}[n(\vec{r})] - E_H[n(\vec{r})] \]
Alternative Exact Definition

Exact XC interaction is unknown

Within DFT we can write the exact XC interaction as

\[
E_{xc}[n] = \frac{1}{2} \iiint n(r) \frac{n_{xc}(r,r')}{|r - r'|} \, dr \, dr'
\]

This would be excellent if only we knew what \( n_{xc} \) was!

This relation defines the XC energy.

It is simply the Coulomb interaction between an electron at \( r \) and the value of its XC hole \( n_{xc}(r,r') \) at \( r' \).
Properties of XC functional

- Although exact form of XC functional unknown, it must satisfy certain properties

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- *Only for occupied orbitals.
## Properties of XC functional

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- **XC hole** is the displaced charge that forms round a point test charge.
- Sum of displaced charge should be the negative of the charge on the test charge.
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- Hartree energy is coulomb interaction of classical charge.
- Contains interactions between electron and itself which are unphysical.
- XC functional should correct this.

*Only for occupied orbitals.
Properties of XC functional

- XC potential should jump discontinuously when infinitesimal amount of charge added to system with integer electrons.

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- For finite systems, XC potential should decay as 1/r at long ranges.
- Orbitals should decay with individual exponents. This is not the case with LDA and GGA.

*Only for occupied orbitals.
Generalities

• All functionals are approximations
  Reports of ‘Failures of DFT’ are actually reports of a failure of the XC functional

• No functional (so far) is accurate(?) for all properties of interest
  No matter what functional is ‘invented’ someone will always find a case where it fails

• Any functional can be applied to any electronic structure problem
  In this sense it is ab initio but we use experience and intuition to decide which one to use
Ladder of functionals (LDA)

The simplest XC functional is the local density approximation (LDA)

\[ E^{LDA}_{xc}[n(r)] = \int n(r)\varepsilon^{\text{hom}}_{xc} [n(r)] dr \]

It was used for a generation in materials science, but is not accurate enough for many chemical purposes.

Typical errors
- Over-binds (binding energy too large)
- Underestimates lattice parameters
- Phase stability incorrect order
- Energetics of magnetic materials in error
Ladder of functionals (GGA)

The generalised gradient approximation (GGA) contains the next term in a derivative expansion of the charge density:

\[
E_{xc}^{GGA}[n(r)] = \int n(r) \varepsilon_{xc}^{GGA}[n(r),\nabla n(r)]dr
\]

Typically (but not always) this is more accurate than the LDA.

GGA greatly reduce the bond dissociation energy error, and generally improve transition-state barriers.

But, unlike LDA, there is no single universal form.
Why the GGA?

• LDA depends only on one variable (the density).

• GGAs require knowledge of 2 variables (the density and its gradient).

• In principle one can continue with this expansion.

• If quickly convergent, it would characterise a class of many-body systems with increasing accuracy by functions of 1, 2, 6, ... variables.

• How fruitful is this? Depends on parameterisation used, but it will always be semi-local.
Ladder of functionals (meta-GGA)

Next come the meta-GGAs

Instead of using $\nabla^2 n$ typically the kinetic energy is used (same idea, in principle)

\[
E_{xc}[n(r), \nabla n(r), \nabla^2 n(r)] \quad \text{or} \quad E_{xc}[n(r), \nabla n(r), \nabla^2 \psi(r)]
\]

Various breeds of functionals

Non-empirical functionals

• Such as LDA

• Some GGAs (PW91, PBE, rPBE, WC, PBEsol, …)

• Not fitted to any empirical results

• These come from known exact conditions

• If these conditions are important to your physical value of interest then you should get a reliable result

• These functionals often have systematic failures (and successes!) so their reliability can usually be predicted
Some GGAs


Different fits for *ab initio* GGAs

- PW91 is the first *reasonable* GGA that can be reliably used over a very wide range of materials.

- PW91 contains much of the known *correct* physics of the exchange and correlation interactions.

- PBE is based on PW91 containing the correct features of LDA but the correct (but *hopefully* not important!) features of PW91 that are *ignored* are:
  1. Correct 2\textsuperscript{nd} order gradient coefficients of $E_x$ and $E_c$ in the slowly varying limit.
  2. Correct non-uniform scaling of $\varepsilon_x$ in the limits where $s$ tend to infinity.

- WC is newer - re-parameterisation of PBE.
Charge Differences (LDA-PW91)
Empirical XC functionals

Good(!) empirical (and non-empirical) functionals are widely applicable

None are good at everything, but they are all reasonable for most properties
e.g. PBE is not the best functional for any particular property but is probably
the best, on average for all properties.

Good empirical functionals are usually best for the particular property that
they were designed for
Various breeds of functionals

Over-fitted functionals

• Contain many fitted parameters – usually from a few dozen to hundreds of parameters

• Usually fitted to a particular set of properties of hundreds of molecules made from atoms of low atomic number

• There are many of these in the literature. Beware: every one of these (so far) only works for systems for which they are fitted

• The academic/Accelrys version of Castep does not contain any of these
Hartree-Fock

Exchange is essentially the Pauli exclusion principle

Quantum mechanically, electrons are Fermions hence many-particle wavefunction is anti-symmetric

$$\Psi(r_1, r_2) = -\Psi(r_2, r_1)$$

which after some generalisation we find the energy is

$$E_{X}^{\text{non-local}} = -\frac{1}{2} \sum_{ij,kq} \int \int \psi_{ik}^*(r)\psi_{ik}(r')\psi_{jq}^*(r')\psi_{jq}(r) \frac{drdr'}{|r - r'|}$$

Note: HF can get properties wrong in the opposite direction from DFT
Moving off the ladder: Hybrid Functionals

• If one method over-estimates your value of interest and another under-estimates it, then the answer you want can be obtained by taking a bit of both! (You may notice this is not *ab initio*).

• Leads to a ‘zoo’ of functionals: aesthetically and conceptually unappealing

\[ E_{xc} = \alpha E_{x}^{\text{exact}} + (1 - \alpha) E_{x}^{\text{local}} + E_{c}^{\text{local}} \]
Hybrid functionals

Hybrid Functionals: a few empirical parameters

These include B3LYP, HSE, B88, PBE0

\[ E_{xc} = \alpha E_x^{exact} + (1 - \alpha) E_x^{local} + E_c^{local} \]

Generally a is around 20-25%. \( E_c^{local} \) usually contains parameters

Good answers provided one works with systems ‘close’ to the set of systems for which the functional was fitted.
Functionals with Hubbard U

DFT+U

• What this is not:
  A general method to get the band gap correct for any material

• What this is:
  Fixes a very specific problem that LDA/GGA can get wrong in highly correlated materials
DFT+U

• A brief digression – the Hubbard model:

\[ \hat{H} = -t \sum_{\langle ij \rangle} a_{i\sigma}^+ a_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \]

• 2 limits:
  
  \( t >> U \):  conventional band solid. Total energy minimised by minimising kinetic energy. Delocalised Bloch states.
  
  \( U >> t \):  energy minised by minimising potential energy. Avoid double occupancy of sites – localised states.

• At half-filling, each site has one electron – Mott insulator
DFT+U

• How does this relate to DFT?

\[ \hat{H}_{KS-DFT} = -\frac{\hbar^2}{2m} \nabla^2 + v_{\text{ext}}(\vec{r}) + v_{\text{Hartree}}(\vec{r}) + v_{\text{xc}}(\vec{r}) \rightarrow \sum_{ij} h_{ij} \hat{a}_i^+ \hat{a}_j \]

• With \( v_{\text{xc}} \) from LDA/GGA, we have a mean-field solution

• This is the same for occupied and unoccupied states

• LDA/GGA will not be able to predict a Mott insulator

• LDA/GGA suffers from self-interaction error
- excessive electron delocalisation

• On-site repulsion \( U \) not well-treated: important correlations neglected

• Particularly important for highly localised \( d \) and \( f \) electrons
DFT+U

• In DFT+U split electrons into two subsystems:
  
  - localised $d$ or $f$ electrons described by $\frac{1}{2} U \sum_{i \neq j} n_in_j$
  
  - delocalised $s$ and $p$ electrons described by LDA/GGA

• Introduce new functional:

\[
E_{LDA+U}[n] = E_{LDA}[n] + E_U[n^\sigma] - E_{dc}[n^\sigma]
\]
**DFT+U**

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\]

Hubbard U term: describes localised electrons
DFT+U

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$$E^{LDA+U}[n] = E^{LDA}[n] + E^U[n_i^\sigma] - E^{dc}[n_i^\sigma]$$

Double counting correction: removes contribution from localised orbitals in LDA/GGA functional
DFT+U

\[ E^{LDA+U}[n] = E^{LDA}[n] + E^U[n_i^\sigma] - E^{dc}[n_i^\sigma] \]

Specifying a \( U \) parameter in units of energy completely specifies this interaction

• Can compute from first principles (various schemes)

• Or treat as an empirical parameter - Typical value is 4-5 eV.

• Warning: this method is regularly mis-used (and results published)
DFT+U

\[ E^{LDA+U}[n] = E^{LDA}[n] + E^{U}[n_i^\sigma] - E^{dc}[n_i^\sigma] \]

Specifying a \( U \) parameter in units of energy completely specifies this interaction

- In CASTEP specify in .cell file:
  
  ```
  %block HUBBARD
  Cu 1 d: 2.5
  %endblock HUBBARD
  ```
Back to non-local functionals

• For non-local functionals solve a *generalised* Kohn-Sham problem:

\[-\frac{1}{2} \nabla^2 \psi_i(r) + V^{\text{loc}}(r) \psi_i(r) + \int dr' V^{\text{nl}}(r,r') \psi_i(r') = \varepsilon_i \psi_i(r)\]

• Note: Integral over all space adds to complexity of problem
• Calculations much more expensive than local methods
Another Non-local Functional: screened-exchange

$$E_{xc}^{nl} = -\frac{1}{2} \sum_{ijkq} \iint drdr' \frac{\psi_{ik}^*(r)\psi_{ik}(r')\psi_{jq}^*(r')\psi_{jq}(r)}{|r - r'|} e^{-k_s|r-r'|}$$

• Based on Hartree-Fock
• Non-local correlation included via screening term

The (orbital-dependent) potential is:

$$V_{xc}^{nl} = -\frac{1}{2} \sum_{jq} \frac{\psi_{jq}(r)\psi_{jq}^*(r')}{|r - r'|} e^{-k_s|r-r'|}$$
Plane wave representation

\[ E_{xc}^{nl} = -\frac{2\pi}{V} \sum_{ikjq} \sum_{G,G',G''} \frac{c_{ik}^*(G)c_{ik}(G')c_{jq}^*(G'+G'')c_{jq}(G+G')}{|q - k + G''|^2 + k_s^2} \]

Note:
- Double sum over bands
- Double sum over k-points
- Triple sum over plane waves
- Computationally painful

\[ N_{plwv} \log(N_{plwv})N_{bands}^2N_{kpts}^2 \]

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Non-local: how expensive?

Non-local scales with cut-off as:

$$\sim E_{cut}^2 \log(E_{cut})$$
Scaling with $k$-points

Scales as:

$LDA \sim N_k^2$

LDA is linear with $k$-points
Why bother with this expense?
Example of non-local functionals: Antiferromagnetic FeO

PBE

LDA+U

Castep Workshop: Frankfurt 2012
Example of non-local functionals: Antiferromagnetic FeO

PBE0

sX

Castep Workshop: Frankfurt 2012
Optimised Effective Potential (OEP)

- Recall exchange energy:
  \[ E_x = -\frac{1}{2} \sum_{ikjq} \int \int drdr' \frac{\psi^*_k(r)\psi_k(r')\psi^*_j(r')\psi_j(r)}{|r - r'|} \]

- Hartree-Fock, sX: \textit{non-local} potential

- OEP: find the optimum \textit{local} potential arising from the non-local HF \( E_x \) (i.e. total energy variational w.r.t \( V \))

- Optimised effective potential can be found from solution of
  \[ \sum_{i=1}^{N^\sigma} \int d\mathbf{r}' \psi_i^\sigma*(\mathbf{r}') \left[ V_{xc}^{OEP}(\mathbf{r}') - V_{i,xc}^{\sigma,NL}(\mathbf{r}') \right] G_0^\sigma(\mathbf{r}',\mathbf{r}) \psi_i^\sigma(\mathbf{r}) + cc = 0 \]
Optimised Effective Potential (OEP)

\[ \sum_{i=1}^{N^\sigma} \int d\vec{r}' \psi_i^{\sigma,*} (\vec{r}') \left[ V_{xc}^{\text{OEP}} (\vec{r}') - V_{i,xc}^{\sigma,\text{NL}} (\vec{r}') \right] G_0^{\sigma} (\vec{r}', \vec{r}) \psi_i^{\sigma} (\vec{r}) + cc = 0 \]

Requires sum over all bands
- in principle infinite
- computationally impractical
- represents a serious convergence issue
Optimised Effective Potential (OEP)

\[ \sum_{i=1}^{N_{\sigma}} \int d\vec{r} \psi_i^{\sigma\ast}(\vec{r}') \left[ V_{xc}^{OEP}(\vec{r}') - V_{i,xc}^{\sigma,NL}(\vec{r}') \right] G_0^\sigma(\vec{r}', \vec{r}) \psi_i^\sigma(\vec{r}) + cc = 0 \]

• In CASTEP we use DFPT to avoid calculation of unoccupied states (Hollins, Clark, Refson and Gidopoulo, PRB 85, 235126 (2012))
Optimised Effective Potential (OEP)

- OEP provides ‘better’ KS bandgaps than LDA/GGA
- Superior to HF
van der Waals

- Traditional functionals do not describe van der Waals interactions

- Recent developments now include semi-empirical dispersion corrections

- Known as DFT+D

- Options in Castep include:

- Still open to research and validation tests
van der Waals Implementation

• Implemented for geometry optimisation:
  – Energies
  – Forces
  – Stresses

• Currently available for a subset of the periodic table

• Mainly first row elements

• Not implemented for all functionals

• Example:
Beyond DFT: Quasiparticles

- Many-body perturbation theory: alternative and accurate means of describing electronic excitations

- Quasiparticle states and energies determined from

\[
\left(-\frac{\hbar^2}{2m} \nabla^2 + v_{\text{ext}}(r) + v_{\text{Hartree}}(r)\right)\varphi_i(r) + \int d^3r' \Sigma(r,r';\varepsilon_i^{qp})\varphi_i(r') = \varepsilon_i^{qp} \varphi_i(r)
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  \]

- \(\Sigma(r,r';\epsilon_i^{qp})\) - ‘self-energy’
  - non-Hermitian
  - non-local, frequency dependent
  - incorporates exchange and correlation effects

- Formally, ‘looks like’ KS eqns \textbf{BUT} very different

- How do we solve this?
The GW Approximation

- Take self-energy to be:

\[
\Sigma(r, r'; \epsilon) = \frac{i}{2\pi} \int_{-\infty}^{\infty} d\epsilon' e^{i\epsilon'\delta} G(r, r'; \epsilon + \epsilon') W(r, r'; \epsilon')
\]
The GW Approximation

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\[ \Sigma(r, r'; \varepsilon) = \frac{i}{2\pi} \int_{-\infty}^{\infty} d\varepsilon' e^{i\varepsilon' \delta} G(r, r'; \varepsilon + \varepsilon') W(r, r'; \varepsilon') \]

• Where \( G(r, r'; \varepsilon) \) - Green’s function

\( W(r, r'; \varepsilon) \) - screened Coulomb interaction
The GW Approximation

- What does this describe physically?
The GW Approximation

- Formally, GW is *dynamically screened* Hartree-Fock

- Replacing $W(r, r'; \varepsilon)$ by $\nu(r, r')$ yields Hartree-Fock

- In practice, we calculate corrections to the Kohn-Sham eigenvalues:

  $$\varepsilon_i^{QP} = \varepsilon_i^{KS} + \langle \varphi_i | \Sigma_{GW}(\varepsilon_i^{QP}) - \nu_{xc} | \varphi_i \rangle$$

- Currently being developed and implemented within CASTEP
Some suggestions

• LDA
  – Nice covalent systems
  – Simple metals
• DFT+U
  – Mott insulators and highly correlated materials
• GGA:
  – Molecules
  – H-bonded materials
  – Highly varying densities (d and f states)
  – Some nasty metals
  – Most magnetic systems
• Non-local hybrids and sX:
  – Band gaps (with caution)
  – Some nasty magnetic systems (again, with caution)
• van der Waals
  – Dispersion: DFT+D methods
Conclusions

• Introduced notion of exchange and correlation

• Introduced various flavours of XC functional in CASTEP

• XC functional employed should be dictated by physics under consideration

• There is no ‘golden bullet’: all XC functionals have pros and cons

• New developments: OEP and GW
Acknowledgements

- CDG
- Tom Hollins, Pete Byrne
- EPSRC