

The DFT Song

written by Volker Blum and Kieron Burke

to the tune of “Let It Be” (with apologies to John and Paul)

When I find my model's unpredictable,
Walter Kohn just comes to me,
speaking words of wisdom,
DFTee.

And in my hour of code-debugging,
he stands right in front of meee,
saying “you just gotta learn
your chemistree”.

LSD, PBE,
B3LYP, hee-hee-hee.
Which approximation should I use,
in my DFT?

And when I find my state's degenerate,
I turn next to Mel Levy
Constrained searches work the best
for formality.

In LDA I have some faith,
if my system's running free
But LDA can never give
A dis-Cont-inuit-eee.

DFT, convexity,
Not Thomas-Fermi, nor Hartree-ee
Exact conditions tell the truth,
no fitting need there be.

For though it may be parted
with hybrid E-X-Cee,
Can I trust my answer,
in realitee?

DFT, DFT,
DFT, DFTee.
I thought you were first principles,
DFTee.

And when the broken-hearted gap,
opens up to full degree,
How'll I get the answer,
tell me DFTee?

For though the band gap may be parted,
there's a chance that you will see:
GW is the answer,
thank you, Rex Godbee!

Many bod-eee, not DFT,
Many bod-eee, no densitee,
this must be the answer,
on which we'll all agree!

And when I've found the structure,
there's still a light that shines on me,
So Walter wont let me use,
ground-state DFTee.

And in my hour of darkness,
with van-der-Waals in front of meee,
my graphene comes out bad,
with stupid PBEee.

But now there's Langreth-Lundqvist,
doing even ATPee,
let's all go to medical conferences,
running DFTee.

DFT, DFT,
DFT, DFTee.
I can always find a functional,
to make it all agree.

But when my band gap's tiny,
far to small to see,
I don't like your answer,
DFTee.

To find the optical spectrum,
while staying p'rameter-free,
We must ask a little Gross,
the one called Hardeee.

DFT, 123,
now TD-, DFT
Let's get excitations,
with more skulduggeree.

DFT, DFT,
DFT, DFTee.
It's the weirdest physics,
but makes great chemistreee!