Notes 60(7): Hartree Term at Resonance.

The solution to the Poisson equation:

$$\nabla^2 \phi = -\rho / \epsilon_0 \quad -(1)$$

is:

$$\phi = \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\underline{r}')}{|\underline{r} - \underline{r}'|} d^3 r' \quad -(2)$$

In the Wikipedia article the correct Hartree term should be:

$$\phi_H = \frac{1}{4\pi\epsilon_0} \int \frac{e n_s(\underline{r})}{|\underline{r} - \underline{r}'|} d^3 r' \quad -(3)$$

so:

$$\boxed{\rho_H(\underline{r}') = e n_s(\underline{r})} \quad -(4)$$

where the number density $n_s(\underline{r})$ has the units of inverse metres cubed.

So the resonance equation of ϕ_H in ECE is:

$$\boxed{-\nabla^2 \phi_H + \underline{\omega} \cdot \underline{\nabla} \phi_H + (\underline{\nabla} \cdot \underline{\omega}) \phi_H = e n_s(\underline{r}) / \epsilon_0} \quad -(5)$$

At resonance ϕ_H and $n_s(\underline{r})$ are greatly amplified. The electron - electron repulsion becomes very large and the molecule or material or crystal releases free electrons. So use eq. (5) in density functional code instead of:

$$\nabla^2 \phi_H = -e n_s(\underline{r}) / \epsilon_0 \quad -(6)$$