# PAW Notes

ffr

$$V_{\mathrm{NL}} = \sum_{nm,I} D^{(0)}_{nm} \, |\beta^I_n\rangle\langle\beta^I_m|$$

$n, m$: beta func indices

$\beta^I_n(\mathbf{r}) = \beta_n(\mathbf{r} - \mathbf{R}_I)$

Electron density:

$$n(\mathbf{r}) = \sum_i \left[ |\psi_i(\mathbf{r})|^2 + \sum_{nm,I} Q^I_{nm}(\mathbf{r}) \, \langle\psi_i|\beta_n\rangle\langle\beta_m|\psi_i\rangle \right]$$

Orthonormality conditions:

$$\langle \psi_i | S | \psi_j \rangle = \delta_{ij}$$

overlap operator:

$$S = 1 + \sum_{nm,I} q_{nm} \, |\beta_n^I\rangle\langle\beta_m^I|$$

$$q_{nm} = \int Q_{nm}(\mathbf{r}) \, \mathrm{d}\mathbf{r}$$

KS equation:

$$H \left|\psi_i\right\rangle = \epsilon_i S \left|\psi_i\right\rangle$$

Hamiltonian operator:

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{eff}} + \sum_{nm,I} D^I_{nm} \left|\beta^I_n\right\rangle\left\langle\beta^I_m\right|$$

Screened coefficients:

$$D^I_{nm} = D^{(0)}_{nm} + \int V_{\mathrm{eff}}(\mathbf{r})\, Q^I_{nm}(\mathbf{r})\, \mathrm{d}\mathbf{r}$$

$$E = \sum_n f_n \left\langle \psi_n \left| -\frac{1}{2}\nabla^2 \right| \psi_n \right\rangle + E_{\mathrm{H}}\left[n + n_Z\right] + E_{\mathrm{xc}}\left[n\right]$$

$$|\psi_n\rangle = |\tilde{\psi}_n\rangle + \sum_i \left(|\phi_i\rangle - |\tilde{\phi}_i\rangle\right) \langle \tilde{p}_i | \tilde{\psi}_n \rangle$$

Index $i$: atomic site $\mathbf{R}$, angular momentum $L = (l, m)$, and additional index $k$ for reference energy $\epsilon_{kl}$.

AE partial waves $\phi_i$ are obtained for a reference atom

PS partial waves $\tilde{\phi}_i$ are equivalent to the AE partial waves outside a core radius $r_c^l$ and match continuously onto $\tilde{\phi}_i$ inside the core radius.

Projector functions $\tilde{p}_i$ are dual to the partial waves:

$$\langle \tilde{p}_i | \tilde{\phi}_j \rangle = \delta_{ij}$$

$$n(\mathbf{r}) = \tilde{n}(\mathbf{r}) + n^1(\mathbf{r}) - \tilde{n}^1(\mathbf{r})$$

$$\tilde{n}(\mathbf{r}) = \sum_n f_n \langle\tilde{\psi}_n|\mathbf{r}\rangle\langle\mathbf{r}|\tilde{\psi}_n\rangle$$

Onsite electron densities $n^1$ and $\tilde{n}^1$ are treated on a radial support grid, that extends up to $r_{\mathrm{rad}}$ around each ion.

$$n^1(\mathbf{r}) = \sum_{i,j} \rho_{ij} \langle\phi_i|\mathbf{r}\rangle\langle\mathbf{r}|\phi_j\rangle$$

$$\tilde{n}^1(\mathbf{r}) = \sum_{i,j} \rho_{ij} \langle\tilde{\phi}_i|\mathbf{r}\rangle\langle\mathbf{r}|\tilde{\phi}_j\rangle$$

$\rho_{ij}$ are the occupancies of each augmentation channel $(i, j)$:

$$\rho_{ij} = \sum_n f_n \langle\tilde{\psi}_n|\tilde{p}_i\rangle\langle\tilde{p}_i|\tilde{\psi}_n\rangle$$

Assuming frozen core approximation.

Introduce four quantities that will be used for the description of the core charge density:

$n_c$: charge density of frozen core all-electron wave functions in the reference atom.

$\tilde{n}_c$: partial electronic core density $\tilde{n}_c$ is equivalent to the frozen core AE charge density outside a certain radius $r_{pc}$, which lies inside the argumentation radius. Used in order to calculate nonlinear core corrections

$n_{Zc}$: point charge density of the nuclei $n_Z$ plus the frozen core AE charge density $n_c$:

$$n_{Zc} = n_Z + n_c$$

$\tilde{n}_{Zc}$: pseudized core density, equivalent to $n_{Zc}$ outside the core radius and shall have the same moment as $n_{Zc}$ inside the core region:

$$\int_{\Omega_r} n_{Zc}(\mathbf{r})\,\mathrm{d}\mathbf{r} = \int_{\Omega_r} \tilde{n}_{Zc}(\mathbf{r})\,\mathrm{d}\mathbf{r}$$