

The concept and the form of DCACPs

$$v_{xc}^{\text{extended}} = v_{xc} + \sum_I v_I^{\text{DCACP}}(\mathbf{r}, \mathbf{r}')$$

$$v_I^{\text{DCACP}}(\mathbf{r}, \mathbf{r}') = \sum_{m=-l}^{+l} Y_{lm}(\hat{\mathbf{r}}) p_l(r) \sigma_1 p_l(r') Y_{lm}^*(\hat{\mathbf{r}}')$$

with the projector,

$$p_l(r) \propto r^l \exp(-r^2/(2\sigma_2^2)).$$

$r = |\mathbf{r} - \mathbf{R}_I|$ is the distance from position \mathbf{R}_I of nucleus I. $\hat{\mathbf{r}}$ is the unit vector in the direction of $\mathbf{r} - \mathbf{R}_I$, and Y_{lm} denotes a spherical harmonic. The dispersion corrected atom centered potential (DCACP) has the same analytical form as the non-local part of the pseudopotentials of Goedecker *et al.* We found that only one projector is sufficient to reproduce the desired accuracy and, usually, a high angular momentum component ($l = 3$) is chosen.

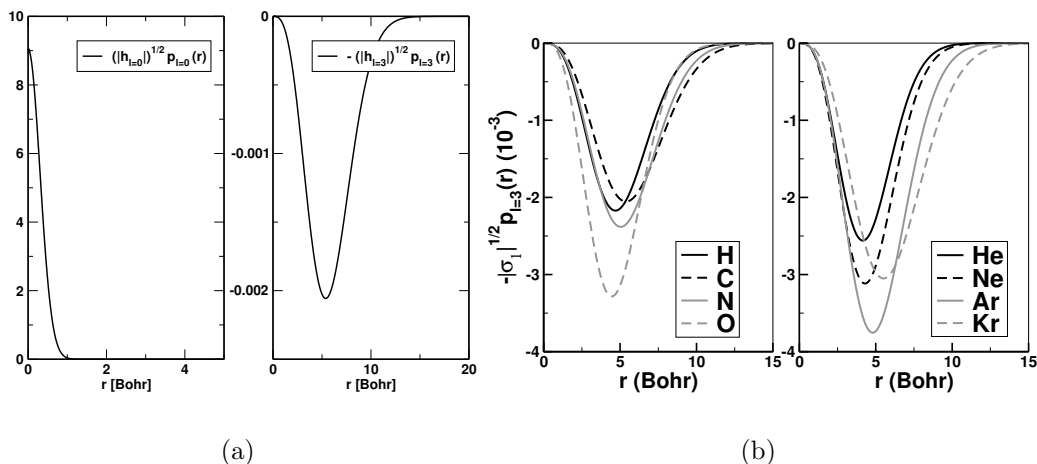


Figure 1: (a) s channel vs DCACP in the form shown in the legend, note the difference in the magnitude; (b) DCACPs complementing the BLYP functional for hydrogen, carbon, nitrogen, oxygen, and the rare gas atoms are shown in the form of $-|\sigma_1|^{1/2} p_{l=3}(r)$ where the projector $p_l(r)$ is proportional to $r^l \exp(-r^2/2\sigma_2^2)$.