

pętla elektronowa

pętla jonowa

Parametry startowe ( $p_i$ ):

$$n_0(\vec{r})$$

$$V_{KS}(\vec{r}) = V_{ext}(\vec{r}) + V_H(n) + V_{xc}(n)$$

$$\left( -\frac{\hbar^2 \nabla^2}{2m} + V_{KS}(\vec{r}) \right) \psi_i(\vec{r}) = \epsilon_i \psi_i(\vec{r})$$

$$n(\vec{r}) = \sum_i |\psi_i(\vec{r})|^2$$

Nie

$$n(\vec{r}) = n_0(\vec{r})$$

Tak

Parametry końcowe ( $p_{out}$ ):

$$E[n(\vec{r}), p_i] = \min$$

Nie

Tak