

# Optimización de la estructura electrónica del átomo de Be

A. Mendez

October 10, 2019



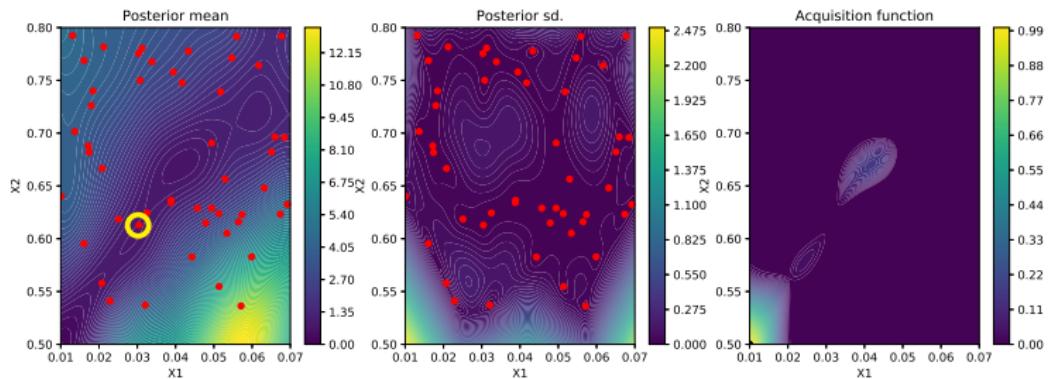


# Variables importantes en la optimización de Be

- ▶ Configuraciones en CI
- ▶ Tipo de potencial modelo  $V_{nl} \rightarrow$  parámetros  $\lambda_{nl}$
- ▶ Potencial de polarización  $V_{\text{pol}}(r) \rightarrow$  parámetros  $\alpha, r_{\text{cut}}$

# Optimización del potencial de polarización

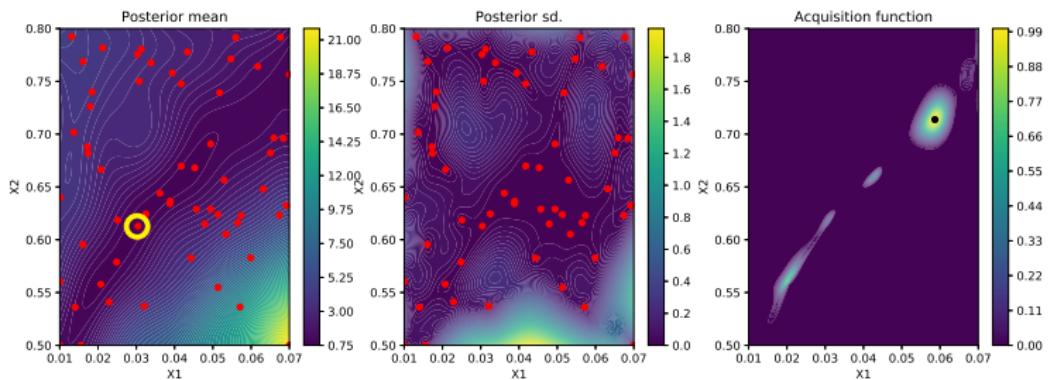
*initer = 50 & maxevals = 0*



$$J_{\min} = 0.8898 \text{ at } \alpha, r_{\text{cut}} = [0.0304, 0.6129]$$

# Optimización del potencial de polarización

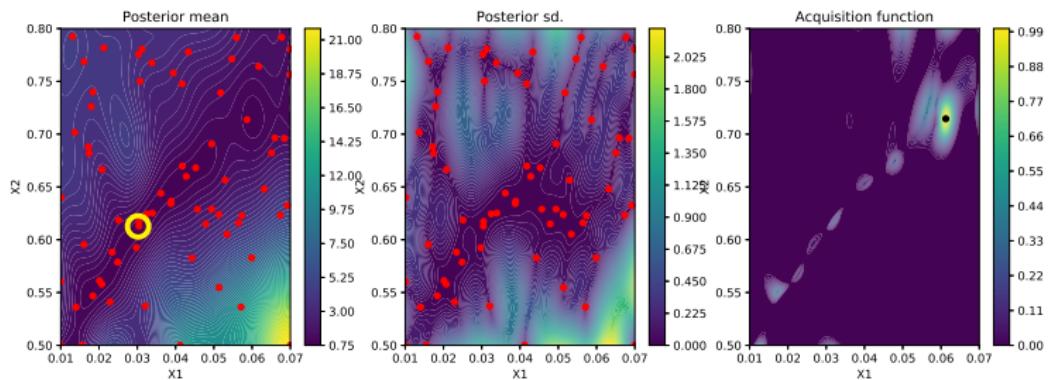
*initer = 50 & maxevals = 10*



$$J_{\min} = 0.8898 \text{ at } \alpha, r_{\text{cut}} = [0.0304, 0.6129]$$

# Optimización del potencial de polarización

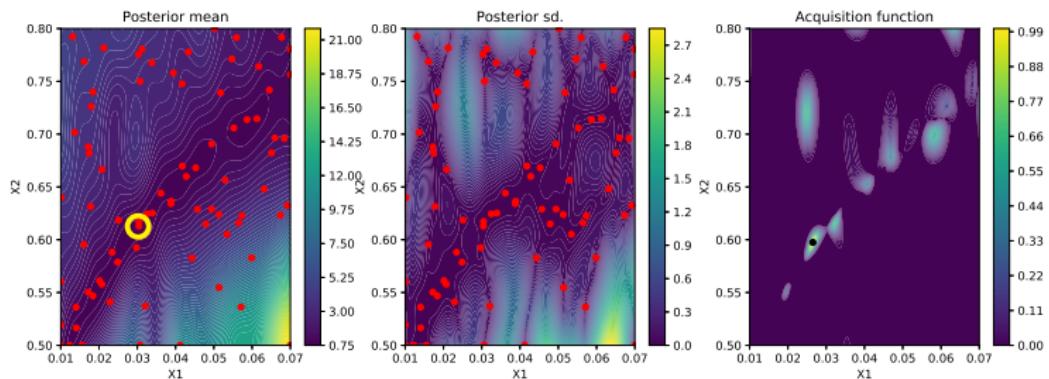
*initer = 50 & maxevals = 20*



$$J_{\min} = 0.8898 \text{ at } \alpha, r_{\text{cut}} = [0.0304, 0.6129]$$

# Optimización del potencial de polarización

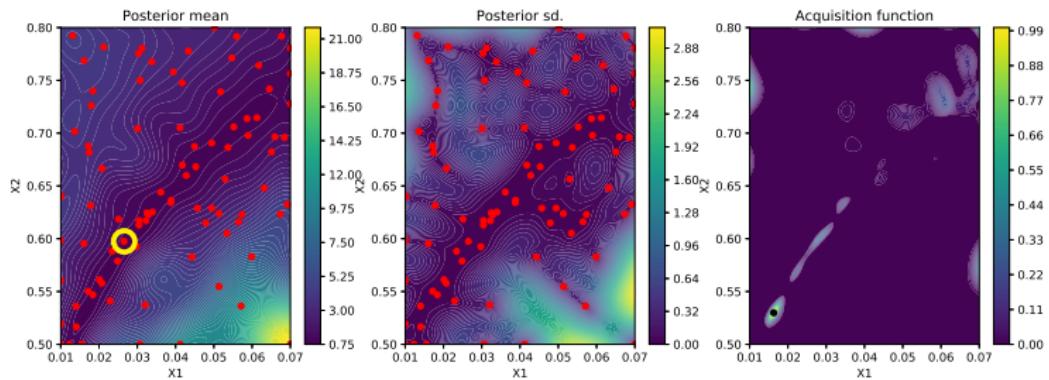
*initer = 50 & maxevals = 30*



$$J_{\min} = 0.8898 \text{ at } \alpha, r_{\text{cut}} = [0.0304, 0.6129]$$

# Optimización del potencial de polarización

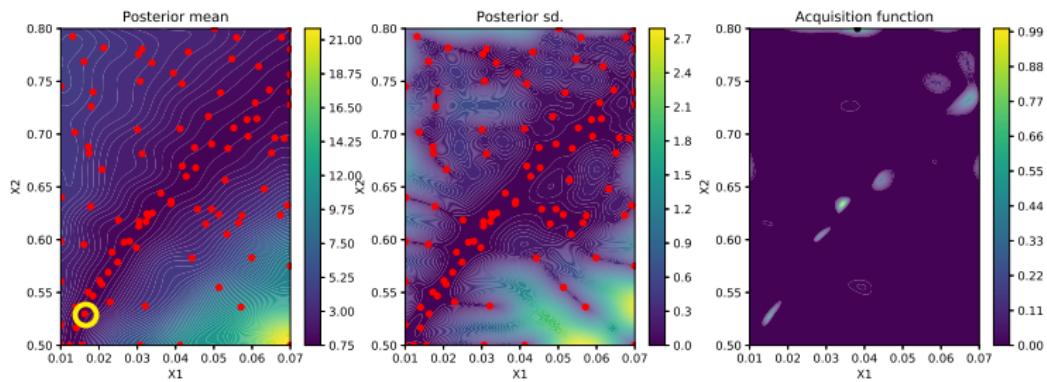
*initer = 50 & maxevals = 40*



$$J_{\min} = 0.8878 \text{ at } \alpha, r_{\text{cut}} = [0.0265, 0.5975]$$

# Optimización del potencial de polarización

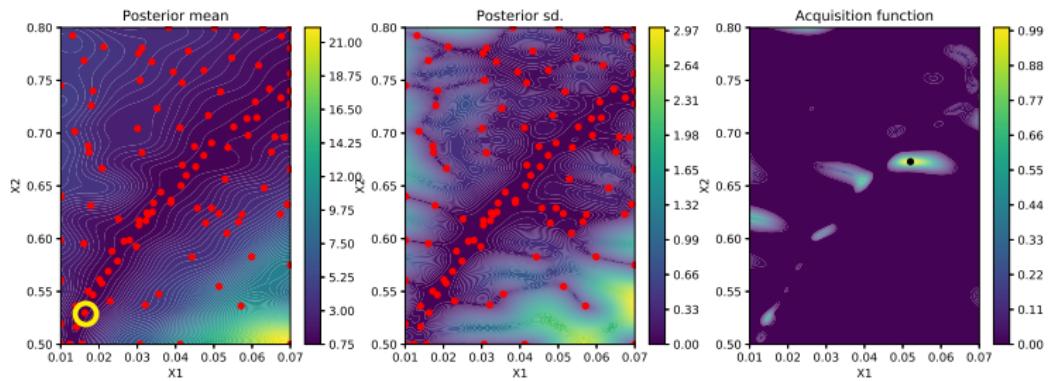
*initer = 50 & maxevals = 50*



$$J_{\min} = 0.8804 \text{ at } \alpha, r_{\text{cut}} = [0.0163, 0.5299]$$

# Optimización del potencial de polarización

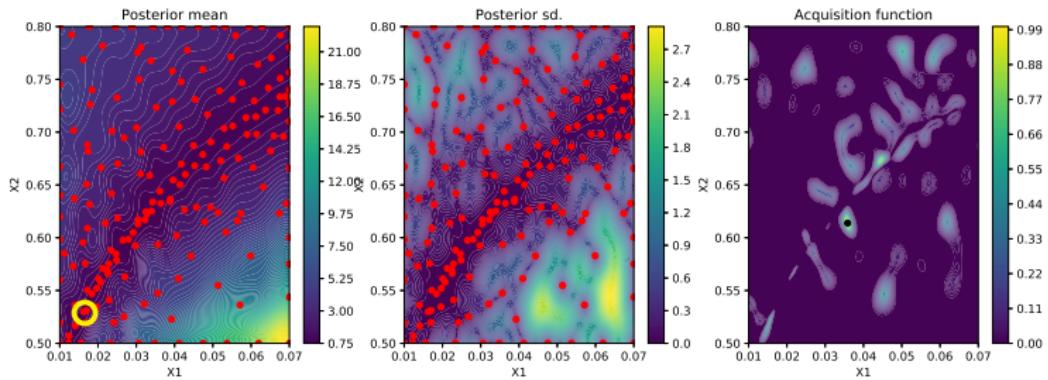
*initer = 50 & maxevals = 60*



$$J_{\min} = 0.8804 \text{ at } \alpha, r_{\text{cut}} = [0.0163, 0.5299]$$

# Optimización del potencial de polarización

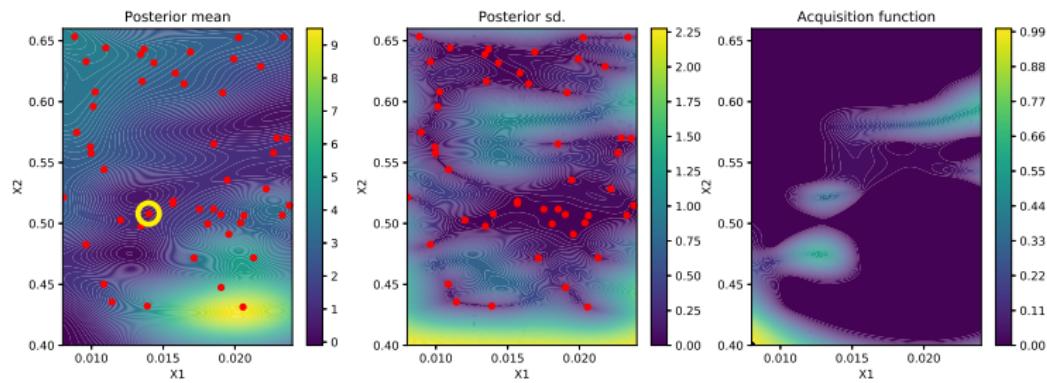
*initer = 50 & maxevals = 130*



$$J_{\min} = 0.8804 \text{ at } \alpha, r_{\text{cut}} = [0.0163, 0.5299]$$

# Optimización del potencial de polarización - parte 2

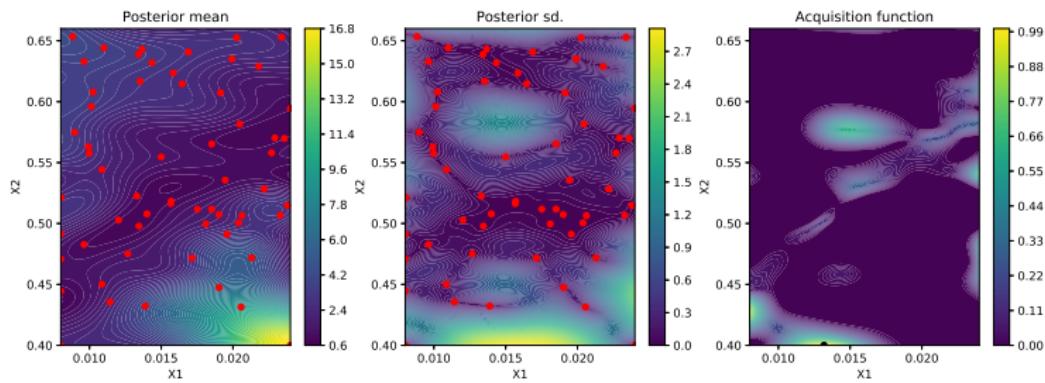
*initer = 50 & maxevals = 0*



$$J_{\min} = 0.8785 \text{ at } \alpha, r_{\text{cut}} = [0.0140, 0.5079]$$

# Optimización del potencial de polarización - parte 2

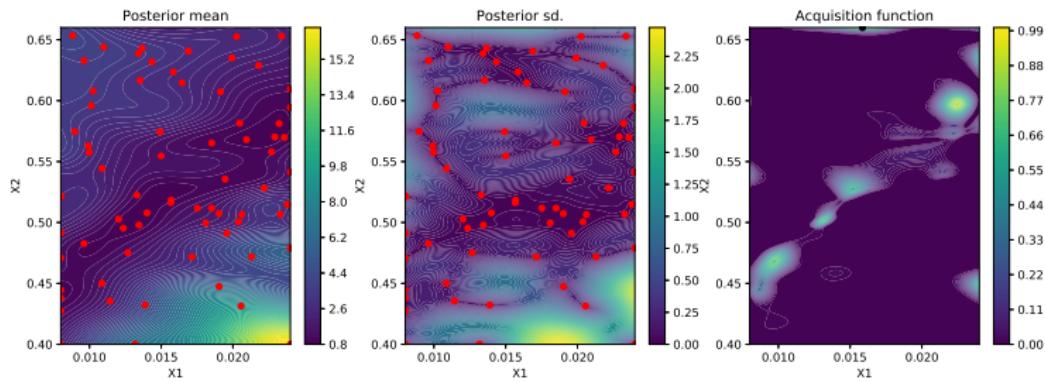
*initer = 50 & maxevals = 10*



$$J_{\min} = 0.8737 \text{ at } \alpha, r_{\text{cut}} = [0.0080, 0.4446]$$

# Optimización del potencial de polarización - parte 2

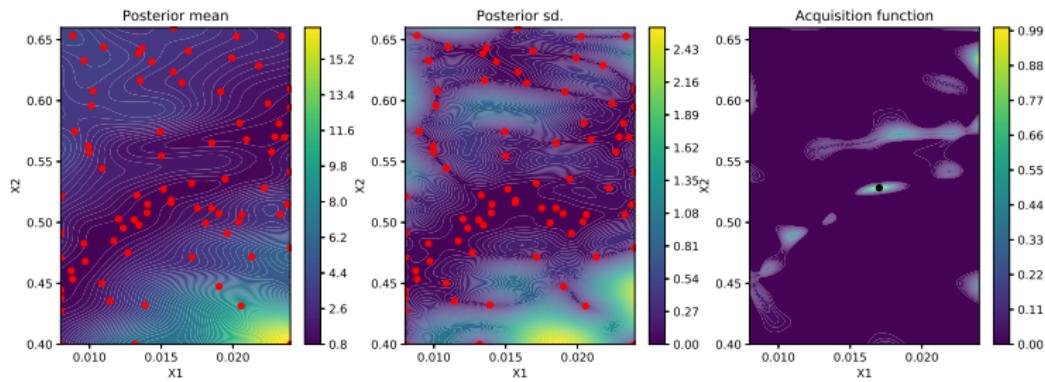
*initer = 50 & maxevals = 20*



$$J_{\min} = 0.8737 \text{ at } \alpha, r_{\text{cut}} = [0.0080, 0.4446]$$

# Optimización del potencial de polarización - parte 2

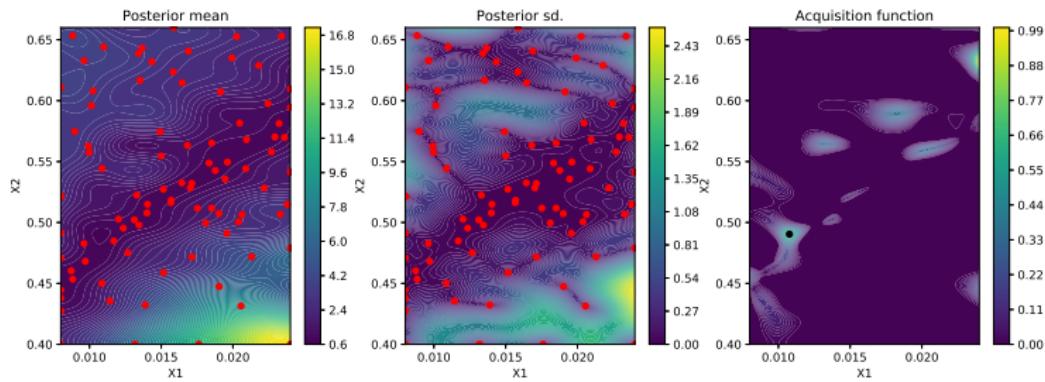
*initer = 50 & maxevals = 30*



$$J_{\min} = 0.8737 \text{ at } \alpha, r_{\text{cut}} = [0.0080, 0.4446]$$

# Optimización del potencial de polarización - parte 2

*initer = 50 & maxevals = 40*



$$J_{\min} = 0.8737 \text{ at } \alpha, r_{\text{cut}} = [0.0080, 0.4446]$$



