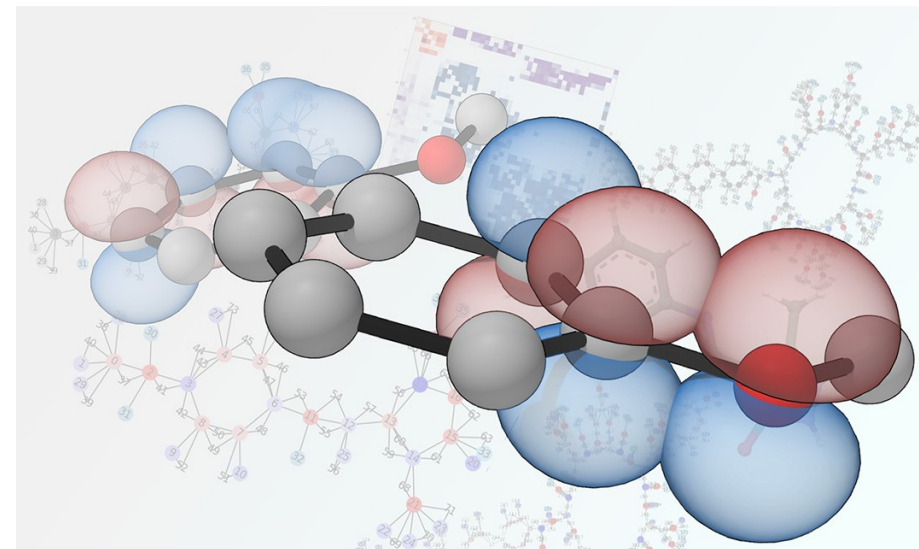


## Aula 13 – Modelos de Solventes Contínuos

Ref: Artigos Citados

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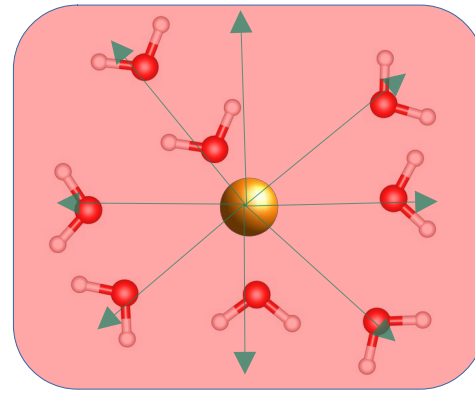
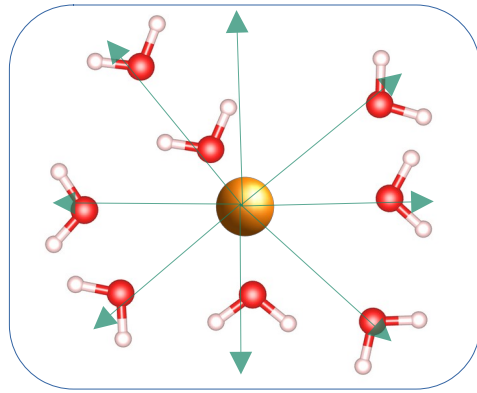
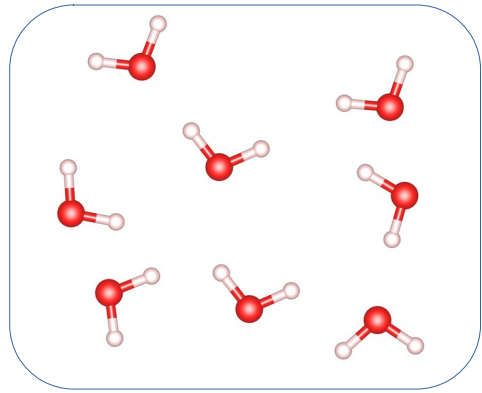


$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \hat{H} |\Psi\rangle$$

$$|\Psi\rangle = |\psi\rangle e^{-iEt/\hbar}$$

$$\hat{H} |\psi\rangle = E |\psi\rangle$$

# Polarização de um meio



Unidades gaussianas  
 $4\pi\epsilon_0 = 1$

$$\rho_t = \rho + \rho_{\text{pol}}$$

cargas ligadas - induzidas

Momento de dipólo por unidade de volume  $\mathbf{P} = \frac{d\mathbf{p}}{dV}$

Polarização  $\mathbf{P} = \epsilon_0 \chi \mathbf{E}$

Suscetibilidade elétrica

Campo Elétrico no meio  $\mathbf{D} = \mathbf{E} + \mathbf{P}$

Equações de Maxwell (meio)

$$\nabla \cdot \mathbf{D} = 4\pi\rho$$

$$\nabla \times \mathbf{D} = 0$$

Equações de Maxwell (vácuo)

$$\nabla \cdot \mathbf{E} = 4\pi\rho_t$$

$$\nabla \times \mathbf{E} = 0$$

$\epsilon = (1 + \chi_e)$  Permissividade elétrica ou constante dielétrica

# Potencial Eletrostático num meio dielétrico

$$\mathbf{D}(\mathbf{r}) = \epsilon(\mathbf{r})\mathbf{E}(\mathbf{r}) \longrightarrow \nabla \cdot \mathbf{D} = 4\pi\rho \longrightarrow$$

$$\mathbf{E} = -\nabla\phi \longrightarrow$$

## Potencial Eletrostático

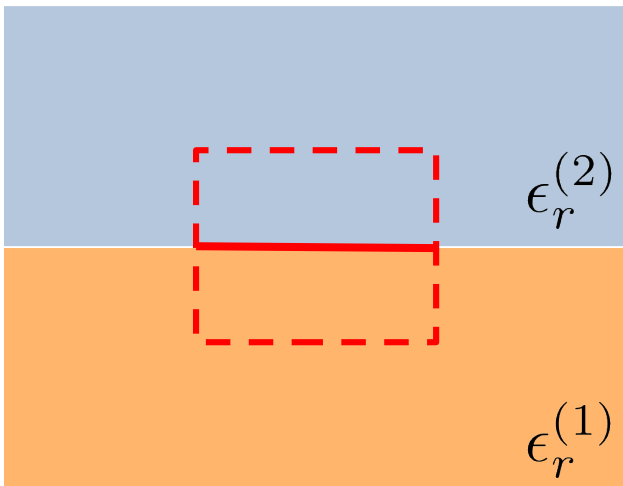
$$\nabla \cdot [\epsilon(\mathbf{r})\nabla\phi(\mathbf{r})] = -4\pi\rho$$



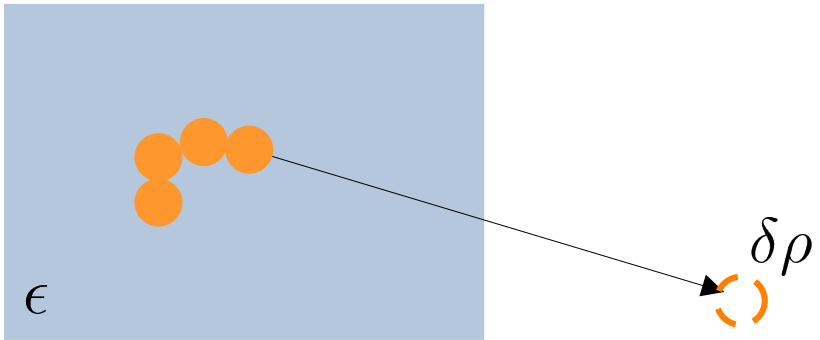
## Condições de contorno

$$\left[ \epsilon_r^{(1)} \nabla\phi_1 - \epsilon_r^{(2)} \nabla\phi_2 \right] \hat{\mathbf{n}} = 4\pi\sigma$$

$$\phi_2 - \phi_1 = 0$$



# Energia de Interação Carga e Dielétrico



$$\delta W = \frac{1}{4\pi} \int_V \delta\rho(\mathbf{r}) \phi(\mathbf{r}) \, d\mathbf{r}$$



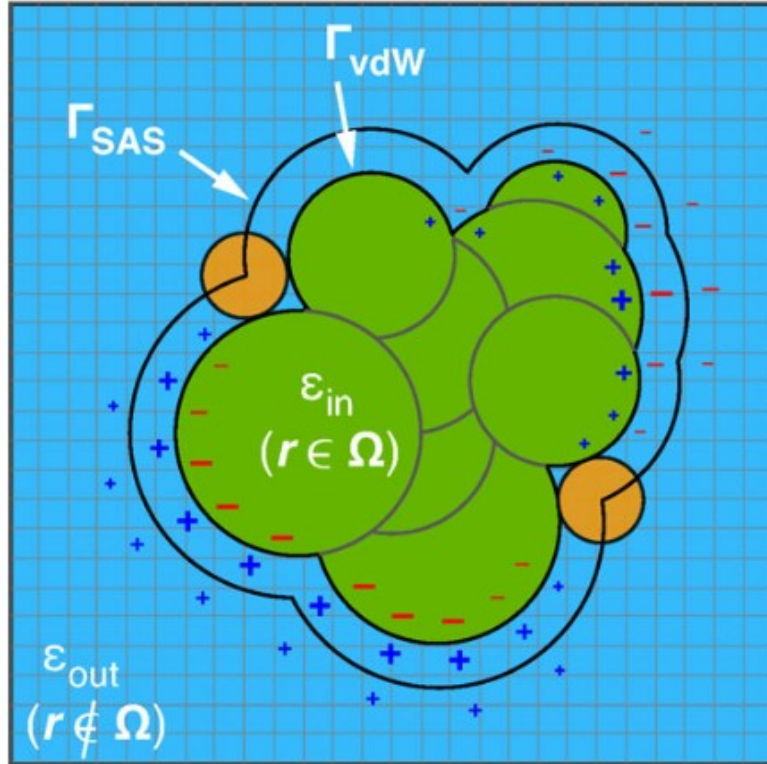
$$\delta W = \delta \left[ \frac{1}{2} \frac{1}{4\pi} \int_V \mathbf{D} \cdot \mathbf{E} \, d\mathbf{r} \right]$$



**Trabalho total feito para colocar  
cargas no dielétrico**

$$W = \frac{1}{8\pi} \int_V \mathbf{D} \cdot \mathbf{E} \, d\mathbf{r}$$

# Molécula em solvente



$$\nabla \cdot [\epsilon(\mathbf{r}) \nabla \phi(\mathbf{r})] = -4\pi\rho$$

reaction field

$$\phi(\mathbf{r}) = \phi^\rho(\mathbf{r}) + \phi_{\text{rxn}}(\mathbf{r})$$

$$\phi^\rho(\mathbf{r}) = \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}'$$

$$\mathcal{G}_{\text{elst}}[\epsilon(\mathbf{r}), \rho(\mathbf{r})] = \int \rho(\mathbf{r}) \phi_{\text{rxn}}(\mathbf{r}) d\mathbf{r}$$

## Energia total

$$\begin{aligned} \mathcal{G}_0[\Psi] &= \langle \Psi | \hat{H}_{\text{vac}} | \Psi \rangle + \mathcal{G}_{\text{elst}} \\ &= \langle \Psi | \hat{H}_{\text{vac}} + \frac{1}{2} \mathcal{R}_0 | \Psi \rangle \end{aligned}$$