Code structure: calculation of matrix elements of H and S. Direct diagonalization

$$\underbrace{\begin{pmatrix} & & \\ & H & \\ & & \end{pmatrix}}_{N \times N} \underbrace{\begin{pmatrix} \\ C \\ \\ \end{pmatrix}}_{N \times 1} = E_{n\vec{k}} \underbrace{\begin{pmatrix} & & \\ & S & \\ & & \end{pmatrix}}_{N \times N} \underbrace{\begin{pmatrix} \\ C \\ \\ \end{pmatrix}}_{N \times 1}$$

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Most important reference followed in this lecture

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The SIESTA method for *ab initio* order-*N* materials simulation

José M Soler[1], Emilio Artacho[2], Julian D Gale[3], Alberto García[4], Javier Junquera[1,5], Pablo Ordejón[6] and Daniel Sánchez-Portal[7]

Goal: solve the one-particle Kohn-Sham Schrödinger-like equation

$$\hat{H}\psi_i(\vec{r}) = E_i\psi_i(\vec{r})$$

Expansion of the eigenvectors in a basis of localized atomic orbitals

$$\psi_i(\vec{r}) = \sum_{\mu} \ldots$$

where the coefficients $c_{\mu i} = \langle \tilde{\phi}_\mu \mid \psi_i \rangle$ **, and** $\tilde{\phi}$ **are the dual orbital of** ϕ **:** $\langle \tilde{\phi} \mid \phi \rangle = \delta$

Introducing the expansion into the Kohn-Shar

$$\sum_{\mu} (H_{\nu\mu} - E$$

$$S_{\nu\mu} = \langle \phi_\nu \mid \phi_\mu \rangle =$$

$$H_{\nu\mu} = \langle \phi_\nu \mid \hat{H} \mid \phi_\mu \rangle =$$