# Density Functional Theory

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#### Molecular electronic Hamiltonian

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$$H = T + V_{ee} + V_{en}$$

$$F = H^{\text{core}} + G$$

$$G_{\lambda\sigma} = \sum_{\lambda\sigma} P_{\lambda\sigma} [2(\mu\nu|\lambda\sigma) - (\mu\lambda|\nu\sigma)]$$

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## Why do we need DFT???

 ${\bf HF\ neglects}\ electron\ correlation$ 

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Electron correlation can be static (multiple near equal energy configurations) and dynamics electron/electron reactions.

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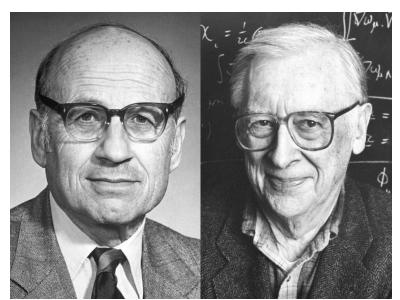
Electron correlation can be static (multiple near equal energy configurations) and dynamics electron/electron reactions.

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This happens because in reality the electrons don't interact with the mean field of the electrons; they interact with all the other electrons.

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### 1998 Nobel Prize



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