FLOW CHART

1. Classical hamiltonian

$$H_{cl} = (1/2M)(p_1^2 + p_2^2) + (1/2m)p^2 + V(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r})$$

↓

2. Complete TISE

$$\mathbf{H} = -(h^2/8\pi^2 M)\,(\partial^2/\partial x_1^2 + \partial^2/\partial y_1^2 + \partial^2/\partial z_1^2 + \partial^2/\partial x_2^2 + \partial^2/\partial y_2^2 + \partial^2/\partial z_2^2)$$
$$- (h^2/8\pi^2 m)\,(\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2) + \mathrm{V}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r})$$

objective: solve for ground state energy E_{tot} and expectation value of proton-proton separation

↓

3. Born Oppenheimer model

(for a particular proton-proton separation R)

$$\mathbf{H}_e = -(h^2/8\pi^2 m)\,(\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2) - (e^2/4\pi\varepsilon_0)(|\mathbf{r}_1 - \mathbf{r}|^{-1} + |\mathbf{r}_2 - \mathbf{r}|^{-1})$$

objective: solve for ground state energy $E_e(R)$ and proton-proton separation R_0

↓

4. Variational solution for $E_e(R)$

Trial wavefunction with adjustable parameters A and B → Find $E_{e,t}(A,B) = (\psi_t, \mathbf{H}_e\psi_t) / (\psi_t, \psi_t)$ → Minimise $E_{e,t}(A,B)$ with respect to A and B → Output is an upper bound to $E_e(R)$

Repeat for different values of R

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5. Add E_{pp} to E_e

to form the BOpp approximation to total energy, E_{tot}

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6. Minimise $E_{tot}(R)$

minimum value found at $R=R_0$

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7. Output minimum E_{tot} and R_0