

Session 2 - Guided problem solving session. Attempt to solve the problem on your place while following your colleague on board. Can you come up with alternative approaches?

1. **Li-H molecule.** Assume a simple molecule model: two neutral non-identical hydrogen-like atoms: $Z_1 = 1$ and $Z_2 = 3$ at finite distance R with non-interacting electrons. Considering only the valance electrons of each atom
 - a) Write a parametrized hamiltonian in the basis of the single-atom valance orbitals. Solve the eigenvalue equation of this hamiltonian and sketch the eigenfunctions.
 - b) Does this hamiltonian commute with the angular momentum operator? Does it commute with the parity operator?

2. **Recap: H-chain.** Consider a hydrogen atom chain with lattice spacing R .
 - a) What is the periodicity of the hamiltonian?
 - b) Using Bloch theorem, write the generic form of the eigenfunctions of this hamiltonian.
 - c) Sketch the band structure of this system.

3. **Li-H chain.** Let us now assume an infinite chain of the simple molecule we have defined earlier where atoms are evenly spaced with distance R .
 - a) What is the periodicity of the hamiltonian?
 - b) Using Bloch theorem, write the generic form of the eigenfunctions of this hamiltonian.
 - c) Sketch the band structure of this system.
 - d) If we replaced all atoms of type 2 with type 1, while keeping everything else the same in this system, how would the band structure change? Comment on the difference of this band structure with the one of the H-chain you have calculated earlier.