

## Tight binding approach

1. Redo the dimerization problem considering  $t$  and  $t'$  for intra-cell and inter-cell hopping. Let  $|t| = 1.5|t'|$ . Plot band structure and mark Fermi energy considering spin degenerate one electron per unitcell. Comment on how would the band structure evolve if they are values are gradually swapped, which essentially would mean that one of the two atoms which came closer gradually shifts away towards the periodic counterpart of the other atom in the next unitcell.

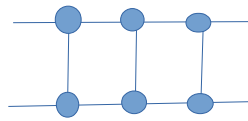
In cartoon we can show this as ...-Bb-Bb-Bb-... becoming ...-bB-bB-bB-... as atom b gradually moves towards right to get closer to atom B in the next unitcell at right. Or B moves towards left to get closer to atom b in the next unitcell at left. B and b are identical atoms.

2. Try tri-merization. Keep all intra and inter cell hoppings same.

You may need (should you need) to use analytical tool like Mathematica to solve for  $E_q$ .

Plot the band structure and understand how bands are getting 'folded' from monomer to dimer to trimer. Note that all are equivalent description of the same system.

3. Consider the ladder system:



Each of the two infinite horizontal lines are referred as 'leg'. Let the intra-leg hopping be  $t$  and the inter-leg hopping be  $t'$ . Let separation between mono-valent atoms along each leg be  $a$  and the inter-leg separation be  $a'$ . Let  $|t| = 1.5|t'|$ . Plot band structure and mark Fermi energy.

Discuss how the system may undergo metal insulator transition as function of  $a/a'$ .