Q1 (4) Would there be a value of k for which the molecule loses its HOMO-LUMO gap (i.e. band gap)? Would that be metallic?

Ans: The HOMO-LUMO gap decreases with increase of length of the molecule (L) and L is proportional to k.

From the plot, for a large value of $k > 100$, the gap asymptotically decreases, however, due to the feature of the molecule, it still maintains a very small (tiny) finite gap and therefore, it cannot be metallic.

So, there won't be any value of k for which the molecule loses its HOMO-LUMO gap in the ground state. So, it won't be metallic.

Q1 (5) Can a metallic state be achieved for larger values of k? Provide your rationale.

Ans: In its ground state, even for a larger value of k, like above (in part 4), the system will have a finite energy gap.

However, when an electron gets excited, may be due to increase in the temperature, the system would achieve metallic character.

Q1 (6) Do you see a transition from molecule to a crystal for larger values of k? How would you justify that?

Ans: Yes, it would form a long chain, leaving the end groups, it certainly forms a crystal that has repeating unit shown in the brackets $[C=C]$.