Lecture 1 - footnote

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Why a basis of a crystal must have $p \times n_b$ balls (ball = atom, ion, or molecule) where n_b is the number of balls in the primitive basis and p is a postive integer:

I give a simple proof that a three atom basis is not possible in graphene. The proof of the general propety stated above is left as an exercise, as all the essential elements of that proof are presented below.

First, note that in graphene there are two different kinds ("colors") of atoms α, β (slide 4 of lecture 1). Any primitive basis needs to have one α atom and one β atom (regardless of in which hexagon and in what part of hexagon these atoms belong). In this notation, we can denote the whole crystal as an infinite series $\alpha\beta\alpha'\beta'\alpha''\beta''$... , where primes and double primes and so on symbolize all possible translations as allowed in the primitive lattice.

Suppose now that a basis of three atoms is possible. It should be readily obvious that this basis should not contain atoms of one color only. The reason is that if one takes the basis as, e.g., $\alpha\alpha'\alpha''$, then by repeating this basis by translation (and by translation only) one can only generate atoms of α color (otherwise we would not have needed to define β color in the first place!). [This observation is the essence of the proof, as you will see below.]

So, the best one can do for a three atom basis is that it should, e.g., look like $\alpha\beta\alpha'$. Let us call this basis B. Let us use the notation B' for another basis, which is a particular translation of B that includes β', i.e., the missing pair of α' in the primitive lattice/basis description. By definition of crystal, B and B' should *not* overlap. One can observe that there is no way one can go from B to B' by translation. There are only three possible translations $T_1(\alpha) = \beta'$, $T_2(\beta) = \beta'$, $T_3(\alpha') = \beta'$. The color changing translations T_1, T_3 are not allowed, since B', by virtue of simply being a repitition of B, has to have two α color atoms and one β color atom. The color conserving translation T_2 is not allowed either, since it implies $T_2(\alpha) = \alpha'$, i.e., B and B' overlap! QED.