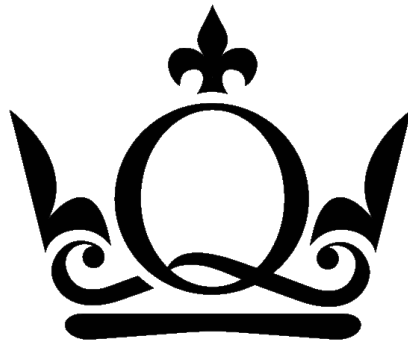


About Lattice Structure

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When a structure can be taken as lattice, it should repeat itself through only translation. In another word, all 'lattice' points in the structure are equivalent to each other, and more importantly, the lattice site is actually an abstract notation, which means the combination of several real points can be taken as a group and the whole group is then taken as the lattice site. Furthermore, the whole lattice structure can be rebuilt following the translation vector:

$$\vec{T} = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3 \quad (1)$$

where \vec{a}_1 , \vec{a}_2 and \vec{a}_3 are the primitive vectors, and u_1 , u_2 and u_3 takes all the integers. Given the primitive vectors and also the coordinates of all the initial atoms within the unit cell, the whole unit cell can be then expanded following the way given by 1. The following animation given in the link illustrates what the unit expansion process looks like: [Click here](#) (If the above link does not show the animation, [Click here](#)). Here it should be pointed out that the definition of primitive vectors – \vec{a}_1 , \vec{a}_2 and \vec{a}_3 – does not depend on the way that is used to describe the lattice structure – it applies to either primitive cell or Bravais unit cell.