Group Theory is a branch of the mathematical field of algebra. One important application, the theory of symmetry groups, is a powerful tool for the prediction of physical properties of molecules and crystals. It is for example possible to determine whether a molecule can have a dipole moment. Many important predictions of spectroscopic experiments (optical, IR or Raman) can be made purely by group theoretical considerations. The qualitative properties of molecular orbitals can be obtained from group theory (whereas their precise energetics and ordering have to be determined by a quantum chemical method). In quantum chemistry group theory can applied to \textit{ab initio} or semi-empirical calculations to significantly reduce the computational cost.

Contributors and Attributions

- Claire Vallance (University of Oxford)
- Thumbnail: Spinning of the high symmetric C\(_{60}\) molecule (CC BY-SA 3.0 Unported; Sponk via Wikipedia)