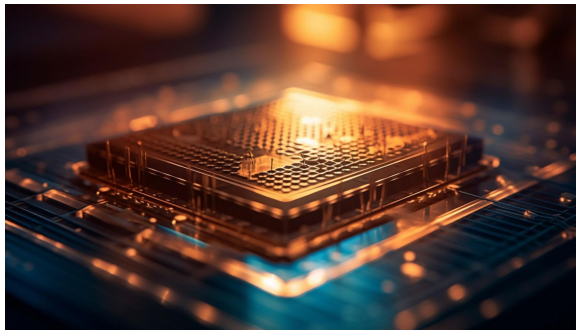
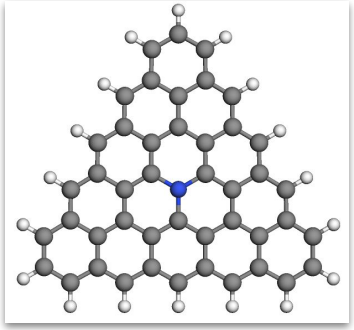
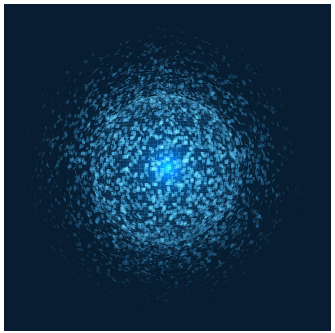
Modelling Qubits with ASAP

In this case study we consider an N doped graphene flake (AZA-Triangulene) to model a spin-Qubit.

Quantum logic gates (basic circuits operating with a few qubits*) enable quantum computers to store more information than classical bits, significantly enhancing memory and processing speed.





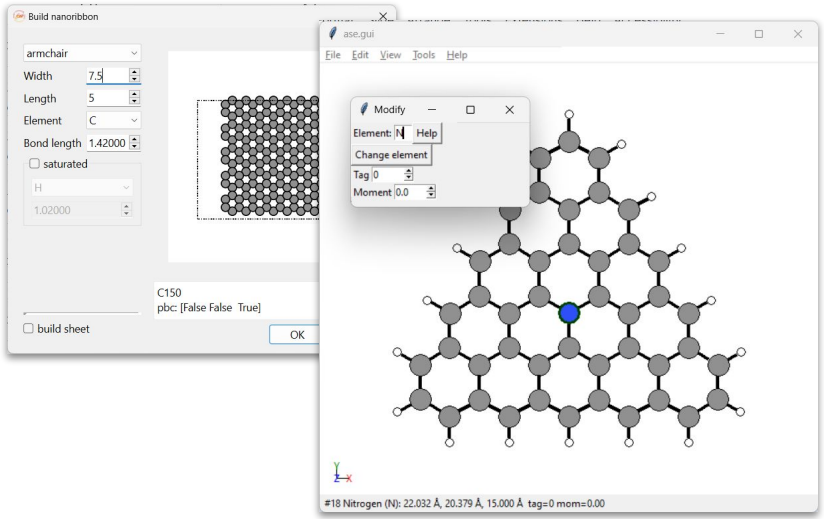


Spin qubits involve manipulating the spin of individual electrons by applying magnetic and electric fields. Magnetic molecule-based qubits offer synthetic control, but reliable solid-state qubits requires the engineering of topologically protected states.

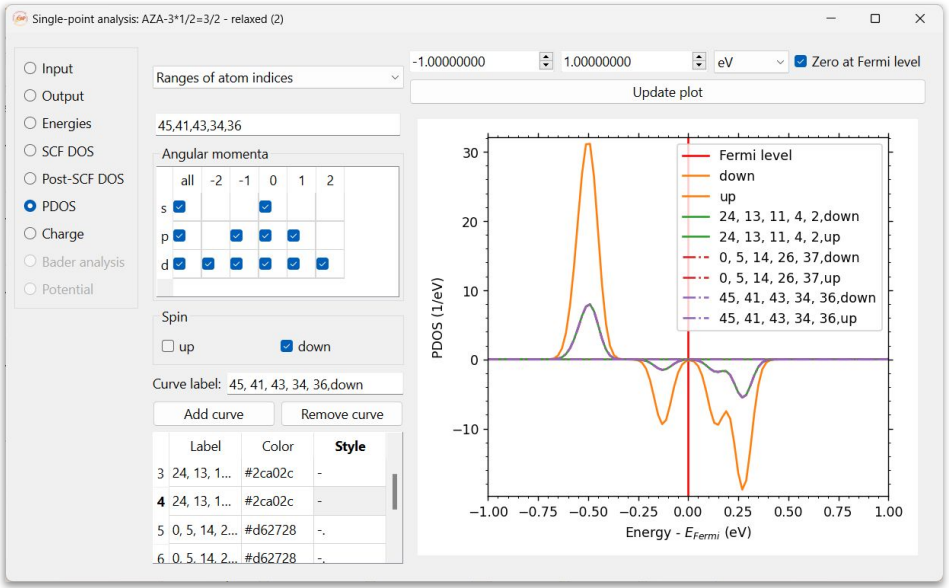
*A qubit (or quantum bit) is the fundamental unit of information in a quantum computer.

Modelling Qubits with ASAP

ASAP's user-friendly graphical interface was used to input parameters for the SIESTA code[1].
ASAP includes workflows specifically designed to extract essential electronic and magnetic properties playing a key role for designing molecular qubits.



ASAP builder is used to build the AZA-Triangulene input structure. Ball-and-stick model representation of the system.



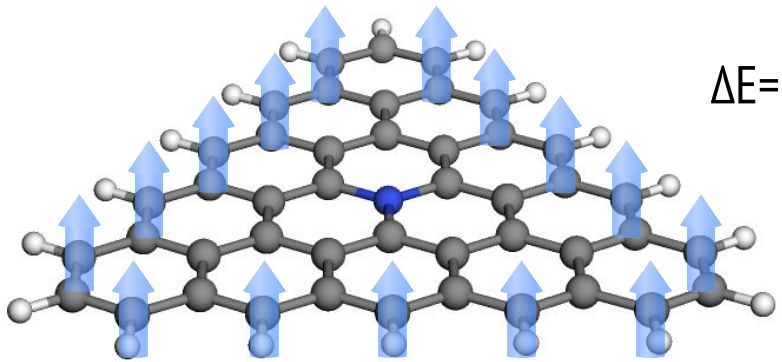
Screenshot of PDOS analysis tool in ASAP

Modelling Qubits with ASAP

In Qubit applications, it is important to know the energy variations (ΔE) associated with distinct spin configurations of the molecule.

Ground state

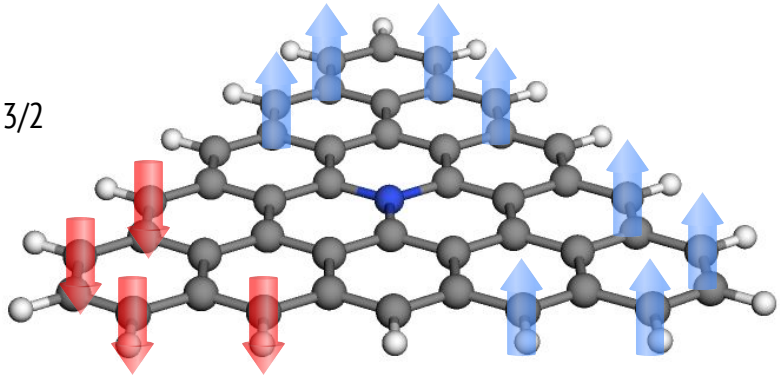
Total Spin: S=3/2



$\Delta E = E_{1/2} - E_{3/2}$

HIgher energy spin configuration

Total Spin: S=½

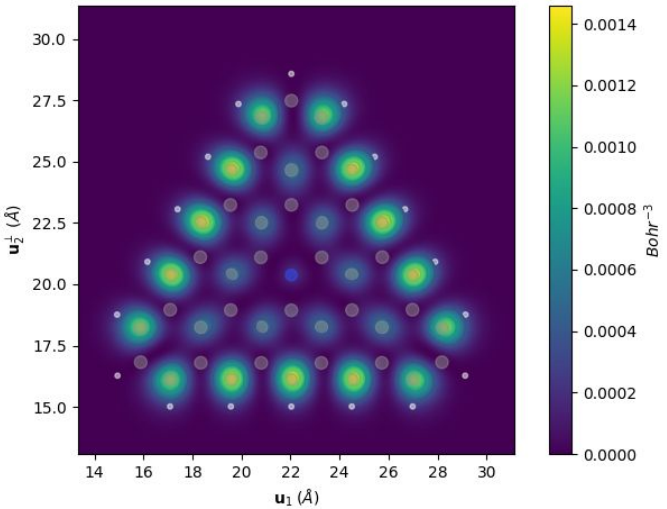


We compute that the energy difference between the two considered spin configurations for AZA-Triangulene is 92meV.

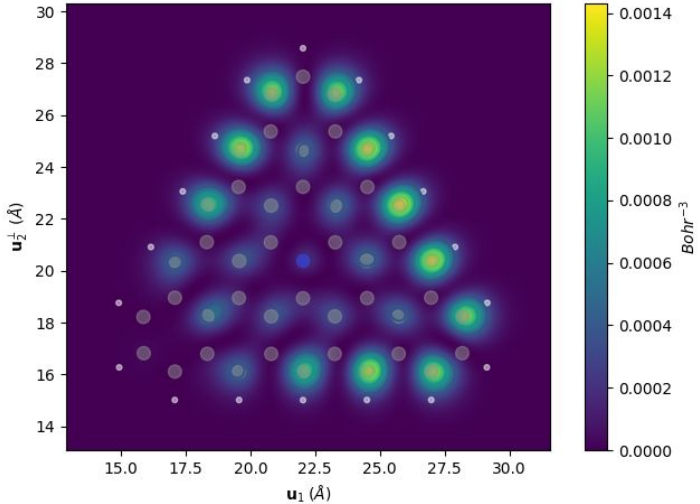
ASAP workflow

ASAP also enables the computation and visualisation of the Local Density of States (LDOS), providing insights into the spin distribution within the system at a selected energy level.

S=3/2



S=1/2



The plots of LDOS spin-up occupied levels close to the Fermi energy show the different electron localization at the zigzag edges of the molecule for the two spin configurations.

Request a trial version of ASAP.

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