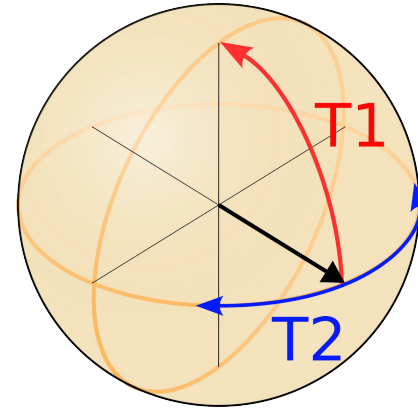


SOC-Driven Anisotropy in atomic-scale Qubits

In quantum information systems, two key timescales define the performance and reliability of a qubit*: The relaxation time (T_1) and the coherence time (T_2).

→ T_1 is the time a qubit stays in its excited state before releasing energy and returning to its ground state, due to interactions with the surrounding environment.

→ T_2 is the time the qubit retains its quantum phase coherence, even without energy lost. It is limited by both relaxation and noise-induced phase fluctuations.



T_1 and T_2 determine how long a qubit can function reliably, and how many operations can be performed before quantum information degrades. Improving them is key to scalable, robust quantum technologies.

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

Estimating T_2 Through Electronic Structure Simulations

Directly computing T_1 and T_2 is challenging, as they depend on dynamic and environmental interactions. In particular, DFT is static and cannot directly capture energy dissipation processes like T_1 or T_2 .

T_2 can be indirectly estimated by analyzing magnetic properties that affect a system's sensitivity to noise and perturbations impacting quantum coherence:

- Spin-orbit coupling (SOC) effect
- Magnetic Anisotropy Energy (MAE)

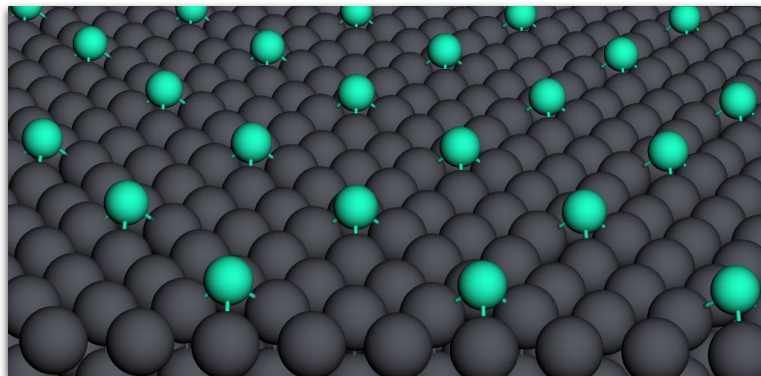
DFT calculations provide insights into qubit stability and coherence, guiding the design of more robust quantum systems.

Role of Spin–Orbit Coupling (SOC) and Magnetic Anisotropy

SOC links an electron's spin to its orbital motion, creating magnetic anisotropy; a directional dependence of magnetic properties.

This anisotropy stabilizes qubit's spin states by protecting them from environmental noise and thermal fluctuations. Strong magnetic anisotropy reduces unwanted transitions, improving both T_1 and T_2 .

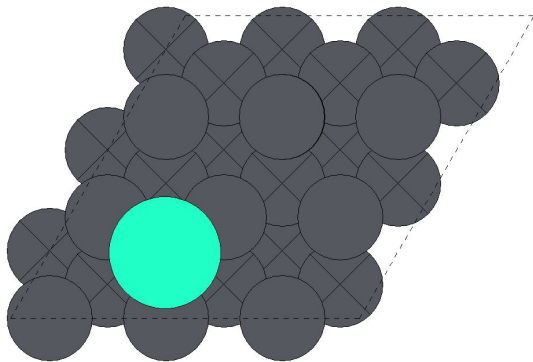
By incorporating SOC effects, simulations can predict how robust a qubit's spin state will be, guiding the design of systems with longer quantum coherence.



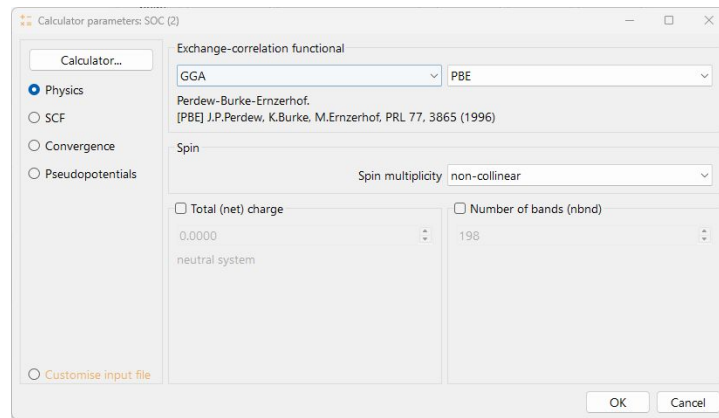
SOC-Driven Anisotropy in atomic-scale Qubits

In this study, we used the user-friendly graphical interface ASAP to compute magnetic properties of Dy/Pd(111), an ideal platform for atomic-scale magnetic systems due to its symmetry and electronic structure.

Dy (heavy rare-earth element with localized 4f electrons) exhibits strong relativistic effects, making SOC a key factor in its magnetic behavior.



Screenshot of ASAP's Builder tool used to construct the Dy/Pb(111) system. Ball model system representation, Dy atom in cyan and Pb atoms in grey.



Parameter setup interface in ASAP-SQ for QE input file generation.^[1]

Our analysis focuses on relative **trends in magnetization** and anisotropy, rather than absolute values*, to provide qualitative insights into the system's behavior.

- The Pb(111) substrate strongly reduces Dy's magnetic moment through hybridization and spin-orbit interactions, altering the balance between spin and orbital contributions and modifying the magnetic anisotropy.
- Spin-orbit coupling can reduce the total magnetization by inducing non-collinear spin arrangements, where misaligned spin components partially cancel each other.

*Absolute magnetization values are underestimated due to lack of pseudopotentials combining full SOC and LDA+U for Dy 4f electrons in Quantum ESPRESSO.

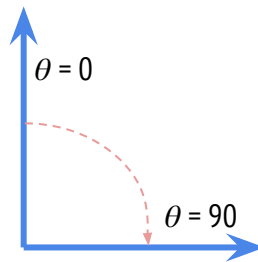
SOC-Driven Anisotropy in atomic-scale Qubits

We compute the Magnetic Anisotropy Energy (MAE) for Dy/Pb(111).

MAE is crucial for magnetic qubit stability. A high MAE means the magnetic moment prefers a specific direction, helping protect quantum states from thermal and external disturbances.

Results reveal a significant MAE exclusively with SOC, highlighting its crucial role in stabilizing the qubit's spin orientation.

In this study, we found an energy difference of 0.4 meV favoring the spin orientation along $\theta = 0$ (the z direction, perpendicular to the surface).



θ (°)	ΔE (meV)
0	0
90	0.452



Request a trial version of ASAP.

