Towards automatic workflows to accelerate the discovery of quantum materials

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Quantum technologies, including quantum computing and quantum communication, face fundamental challenges due to decoherence and information loss caused by environmental interactions, imposing important limitations in application and scalability of quantum systems.[1,2] One promising approach to mitigate these issues lies in topological materials, which host exotic quantum states that are inherently protected from local perturbations. By leveraging the unique properties of topological phases—such as robust edge states—these materials offer a potential pathway toward fault-tolerant quantum computing and resilient quantum devices.[3]

To overcome the fundamental challenges in quantum technologies then, is critically connected to the search for novel materials with tailored electronic, magnetic, and topological properties, which are essential for developing next-generation quantum devices, energy-efficient electronics, and resilient information systems. Advances in computational methods, high-throughput simulations, and machine learning are accelerating the identification of materials with desirable quantum characteristics, such as long coherence times, strong spin-orbit coupling, and intrinsic topological protection.

Among the most attractive platforms for realizing topological properties are two-dimensional (2D) materials.[4,5] These materials exhibit a diverse range of electronic phases, including quantum spin Hall insulators, Chern insulators, and topological superconductors, where topology plays a crucial role in defining their electronic and magnetic behavior. The reduced dimensionality of 2D systems enhances quantum confinement effects and allows for better tunability through external fields, strain, and stacking engineering. This interplay between topology and low-dimensional physics makes 2D materials a fertile ground for exploring novel quantum phases.[6]

Herein, we present a first-principles investigation of topological magnonics in chromium trihalides (CrX_3).[7] We present a rational analysis about the origin of the topological gap in the magnon spectra of CrI_3 according to the competition between the microscopic interactions of atomic orbitals. This complex analysis requires from different physical models and computational packages, such as DFT simulations, Wannier Hamiltonian, Spin models, Montecarlo simulations and spin wave theory, illustrating the potential of building extensive workflows to rationalise the design of new materials.

Motivated by the potential of automatised workflows presented in this illustrative case, we introduce our recent advances in a new platform to automatise materials discovery, aiming to offer flexible simulations of different DFT packages, tight-binding, transport calculations, molecular dynamics, spin models and atomistic simulations. This new platform, aims to use the most recent advances in the field of AI to assist researchers in the exploration and rationalisation of new materials, aiming to contribute to the expansion of the frontiers of knowledge in materials science and quantum technologies.

Figures

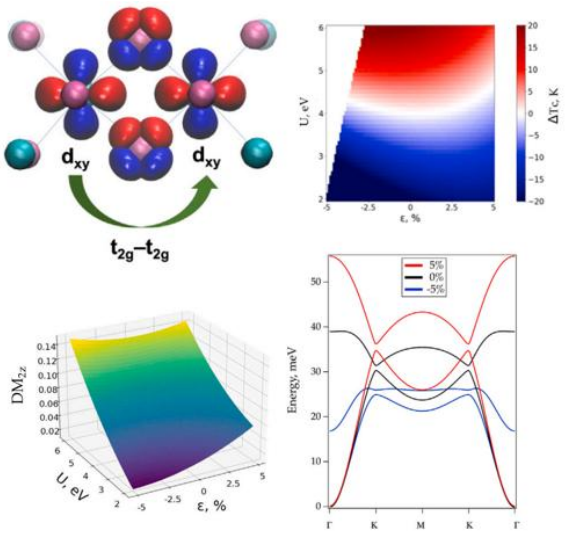

Figure 1. Analysis of a 2D material involving different models and packages.

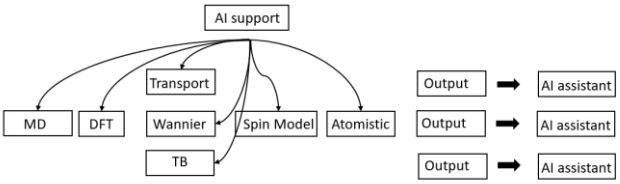

Figure 2. Scheme of an automatized workflow assisted by AI.

References

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