A comprehensive framework for quantum simulations of crystal structures using plane-wave and Wannier function-based methods

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High-strength aluminium alloy, such as Al-Mg based alloys, are widely employed in aerospace as structural materials. Even though they show astonishing good fatigue resistance, they are also sensitive to hydrogen embrittlement (HE). An exposure to this phenomenon leads to loss of tensile strength and accelerated fatigue crack growth, but the mechanism is not yet fully understood. A proposed one, is the hydrogen enhanced decohesion, where it gathers at high triaxial stress location [1,2]. Since the mechanism is not well known, it poses a significant challenge in term of its theoretical understanding but also how to experimentally prevent it. A precise computational characterization of electronic structures is essential to deepen our understanding of this process [1-3].

Over the past decades, *ab-initio* calculations – such as Density Functional Theory (DFT) – try to describe crystal structures. However, solving the Schrödinger equation to obtain ground-state properties presents exponential scaling challenges. Even though DFT makes more feasible calculations for many-body systems, it struggles with strongly correlated systems. Recent advancements in quantum computing offer potential solutions to overcome this exponential scaling barriers. Despite progress, current quantum algorithms often exceed the capabilities of modern hardware, with deep circuits leading to errors and optimization challenges in large-scale problems. An alternative is to use hybrid quantum-classical algorithms which are based on the main advantages of both quantum and classical simulations.

We present an interface between the plane-wave based DFT software, Quantum ESPRESSO (QE) and Qiskit [4]. Our framework is a three steps method. The electronic structure is obtained with QE. We define an active space with the Kohn-Sham orbitals, calculate the one-electron and two-electron integrals for the active space, while the remaining electrons are frozen. The ground-state wavefunction is found using the VQE algorithm [5]. Since plane-wave methods struggle in describing local properties such as defects, in our case hydrogen. By using the software Wannier90[6], it is possible to project the Kohn-Sham plane-waves based orbital onto a basis set of Wannier orbitals. Thus, we can express the electronic Hamiltonian in both basis sets. To this framework, population analysis can be performed by calculating the Bader charges of the crystal structure [7]. This optimized approach aims to deliver accurate descriptions of a crystal structure by providing simultaneously an enhanced electronic ground-state wave-function and of the bader charges located at each atom.

References

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