O 20: Electronic structure theory – Poster

Time: Monday 18:00–20:00 Location: P2

O 20.1 Mon 18:00 P2

From Wannier Functions to Optimal Local Orbitals: A Systematic Approach for Accurate Wavefunction Representation — •Ann Chantal Goutier and Michael Schüler — Laboratory for Materials Simulations, Paul Scherrer Institut, Villigen PSI 5232, Switzerland

Electronic structure calculations in solids are commonly carried out using DFT algorithms with large initial basis sets. These basis sets are compressed into smaller basis sets localised around atoms to calculate quantities of interest. It is desireable to be able to do this conversion with only minimal loss of accuracy. The most common algorithm for this is Wannierisation, a unitary transformation of the Hamiltonian into a space of maximally localised wave functions. Wannierisation preserves the Hamiltonian exactly, but Wannier wave functions cannot be used to construct eigenstates explicitly.

We propose new methods to create Local Orbitals directly, building on the idea of Smart Local Orbitals (Gandus, 2020). Our methods maximise the projectability of the Local Orbital basis set onto electronic eigenstates. This can be done either by blockdiagonalisation of a projectability operator, or by singular value decomposition of the overlap. It is advantageous as less information about the system is required and the Local Orbital set can be systematically improved by adjusting projectibility cut-offs. We also showcase the impact of variationally optimising the Local Orbital basis with respect to different parameters to further improve the representation of Kohn Sham states within a minimal basis.