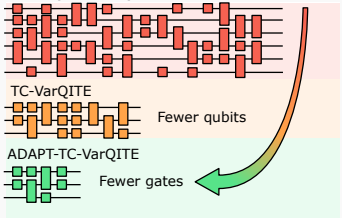
HPC+QC algorithms toolkit to study strongly correlated electron problems

Simulation of bio-chemical transition metal compounds relevant for the **green energy transition**

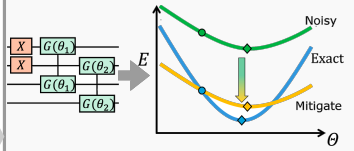
WP1

Resource Reduction

- Accurate calculations for relevant problems on current and future NISQ devices
- Transcorrelation, active spaces, spin-symmetry and adaptive quantum Ansätze

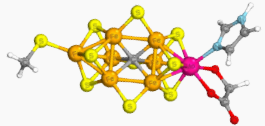


Quantum Error Mitigation



Relevant Applications:

Electronic structure of transition metal compounds



WP2

Algorithms and Software

for relevant insights:

- Electronic properties
- Excited states
- Quantum embedding
- Efficient QC+HPC implementation