Electronic Structure Theory of Complex Materials
Density functional theory-based methods
Many-body perturbation theory

Phenomena
• Weak interactions
• Excited states
• Charge transport

Methodology
• Dispersion-corrected and range-separated hybrid functionals
• GW approximation and Bethe-Salpeter equation approach

Applications to MOFs
• Excited state, transport, and catalytic properties
• Stability and molecular adsorption

Figure 1: CO$_2$-MOF binding geometries for a) Mg-MOF74 and b) Ca-BTT. The unit cell is shown for each MOF. For Mg-MOF74, the primitive cell (one third of the unit cell) is used for all calculations.