Quantum Materials display competing phases with fascinating physical properties, which result from the multiple degrees of freedom in presence (charge, spin, orbital, lattice) and from strong electronic correlations. In this talk, I will show how computational methods aimed at the quantum many-body problem can be combined with realistic electronic structure methods in order to shed light on these physical properties, help identify relevant mechanisms and formulate simple effective models. This will be mostly illustrated by rare-earth nickelates, a family of materials which displays a metal-insulator transition which can be controlled by strain, gating or light pulses.