Model Hamiltonians are simplifications of the exact Hamiltonian but which are though to be able to describe the physics of a given system or family of systems. The Heisenberg and the t-J model Hamiltonians are well-known examples broadly used in solid state physics to describe strongly correlated systems such as the high critical temperature superconducting cuprates. However, a weak point of this approach lies in the fact that model Hamiltonians are defined through parameters which are usually fitted to reproduce experimental data. In this talk I will present a bottom-up approach which permits to define well defined model Hamiltonians from accurate quantum chemical calculations based either on explicitly correlated wave functions or on density functional theory. For the latter, new methodological aspects will be presented which show the weak point of this approach.