Abstract: Quantum computers are appealing for their ability to solve some tasks much faster than their classical counterparts. In fact, they have a potential to perform the full configuration interaction (FCI) energy calculations with a polynomial scaling only. This is in contrast to conventional computers where FCI scales exponentially. We provide a detailed description of the quantum version of the FCI method and the results of numerical simulations of the ground and excited state energy calculations of the methylene molecule. We further generalize this method to the relativistic four component regime and show how to efficiently solve the eigenproblem of the Dirac-Coulomb(-Breit) Hamiltonian on a quantum computer. We demonstrate the functionality of the proposed procedure by numerical simulations of computations of the spin-orbit splitting in the SbH molecule. Finally, we propose quantum circuits with 3 qubits and 9 or 10 CNOTs, which implement a proof-of-principle relativistic quantum chemical calculation for this molecule and might be suitable for an experimental realization.