We extend the theory of the Perelman's functionals on smooth compact manifolds to manifolds with isolated conical singularities. For the $\lambda$-functional, this is essentially an eigenvalue problem for a Schrödinger operator with singular potential. We obtain a certain asymptotic behavior of eigenfunctions near the singularities. This asymptotic behavior plays an important role for deriving the variation formulas of the $\lambda$-functional and other applications. Moreover, we show that the infimum of the $W'$-functional over a suitable weighted Sobolev space on compact manifolds with isolated conical singularities is finite, and the minimizing function exists. We also obtain a certain asymptotic behavior for the minimizing function near the singularities. This is a joint work with Prof. Xianzhe Dai.