A hybrid meta functional, revM06, was developed and optimized based on a previous functional revM06-L, leading to improved calculations of transition-metal bond energies, atomic excitation energies, isomerization energies of large molecules, molecular structures, and both weakly and strongly correlated atomic and molecular data, as well as noncovalent interactions, including smoother potential curves for rare-gas dimers.

RevM06 has broader accuracy than either M06 or M06-2X: as a result, the revM06 functional is well suited for applications requiring simultaneously good performance on main-group chemistry, transition metal chemistry, and molecular structure prediction.

The revM06 functional was optimized against 418 atomic and molecular energies and 10 molecular structures of the Minnesota Database 2017. The performance of revM06 was further assessed on 15 non-training datasets.