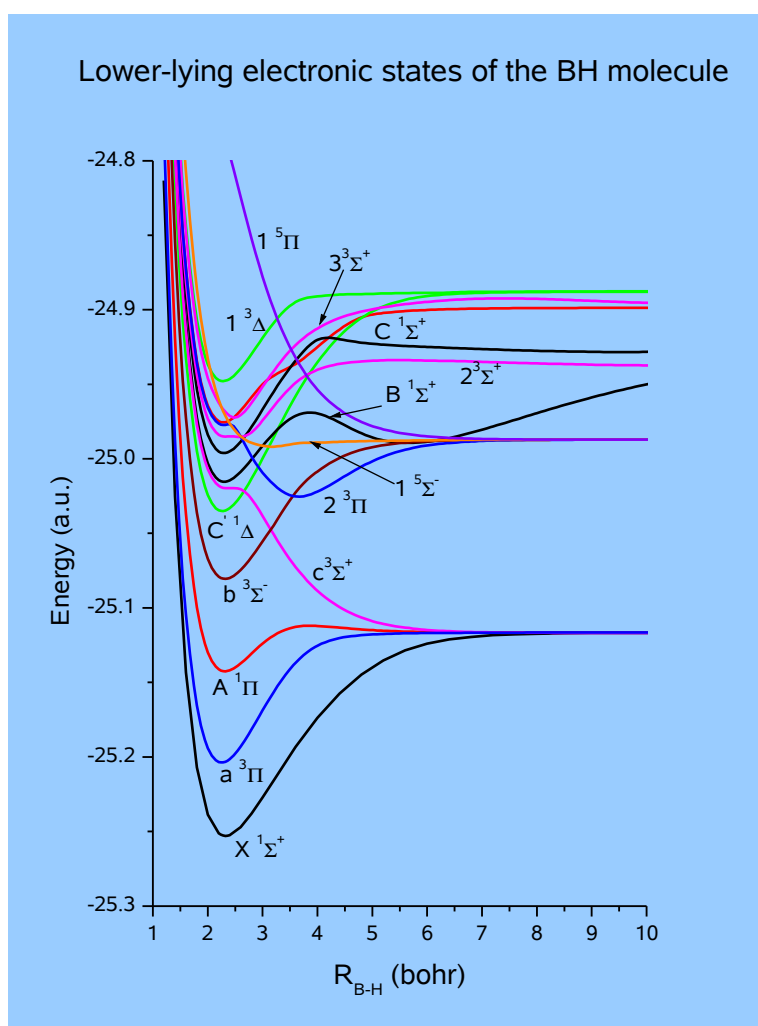


Excited states of molecules. Rydberg spectra, predissociation, autoionization

Excited electronic states of molecules are very important for the chemistry of the atmosphere, the chemistry of the interstellar medium, energy storage, spectroscopy, laser systems, heterogeneous catalysis and the chemistry of molecules on metal and semiconductor surfaces.

Theoretical treatment of the excited states even for simple diatomic molecules has quite different requirements from ground-state treatments. In general, there are excited states of different character, such as valence, Rydberg, charge-transfer etc., and many types of interactions, such as radial, rotational-electronic, spin-orbit etc. that couple them. Multi-reference, large-scale configuration interaction calculations are required for the proper treatment of excited states of molecules, within the Born Oppenheimer approximation, followed by treatments of the non-adiabatic interactions.



In the TPCI, we employ the Multi Reference configuration interaction method (MRDCI) <http://www2.uni-wuppertal.de/FB9/praha/buenker/buenker.html> for the basic electronic structure calculations and coupling matrix elements. Subsequently, calculations are carried out for

- Radiative transitions, bound-bound and radiative dissociation.
- Application of the [complex scaling method](#) for predissociation resonances in multi-state problems and electronic autoionization resonances in diatomic molecules.
- Prediction of the highly excited Rydberg states, spectral perturbations and vibrational autoionization by the [MQDT method](#) in diatomic and triatomic molecules.

At TPCI we have systematically studied by the above methods systems such as the [Rydberg molecules](#) and rare-gas dimers.

Theoretical study of complex systems involving [metal-oxygen bonds](#) and of reactions of oxygen on metal surfaces are part of current activity at the TPCI in the area of excited states of molecules.