

A Look into Ultracold Molecular Physics



Internship at Laboratoire Aime Cotton



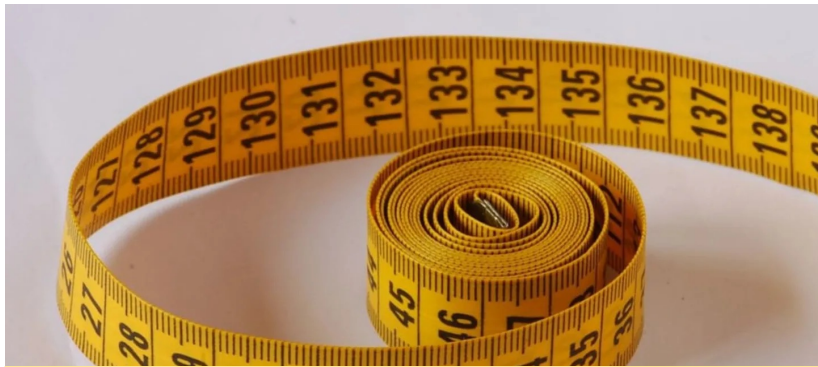
Why Ultracold Molecules?

Molecular Structure

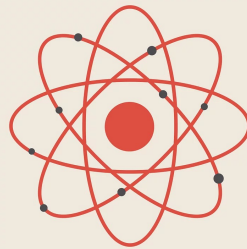
Cooling Molecules (Photoassociation)

Current Applications

Why Ultracold Molecules?



Precise Measurement



Probe New Physics



Controlled Chemical Reaction

Molecular Structure

Time-independent Schrödinger Equation:

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

Hamiltonian:

$$\hat{H} = \hat{T}_N + \hat{T}_e + \hat{V}_N(\vec{R}_i) + \hat{V}_e(\vec{r}_j) + \hat{V}_{Ne}(\vec{R}_i, \vec{r}_j)$$

(\hat{T} is the kinetic term, \hat{V} is the potential term. Subscript N , e , Ne denote to the nuclear, electron, and nuclear-electron terms respectively. R_i and r_j are the position vectors of all the nuclei and electrons respectively.)

Born-Oppenheimer Approximation

- Due to the large difference in the masses of the nucleus and the electron, the time scale of the motion of the electron is negligible compared to that of the nuclei, and the systems of the nuclei and the electrons can hence be decoupled:

$$\Psi = \psi_N(\vec{R}) \times \psi_e(\vec{R}; \vec{r}_i) \quad (\text{Separation of wavefunction})$$

(For a diatomic molecule, \vec{R} denote the relative position of the two nuclei.)

Adiabatic Approximation

- The TISE can be separated into the electronic and nuclear part. The eigenvalue of the electronic wave equation will enter the nuclear wave equation as an electronic potential:

(Electronic wave equation) $\hat{H}_e(\vec{R}; \vec{r}_i)\psi_e(\vec{R}; \vec{r}_i) = E_e(\vec{R})\psi_e(\vec{R}; \vec{r}_i)$

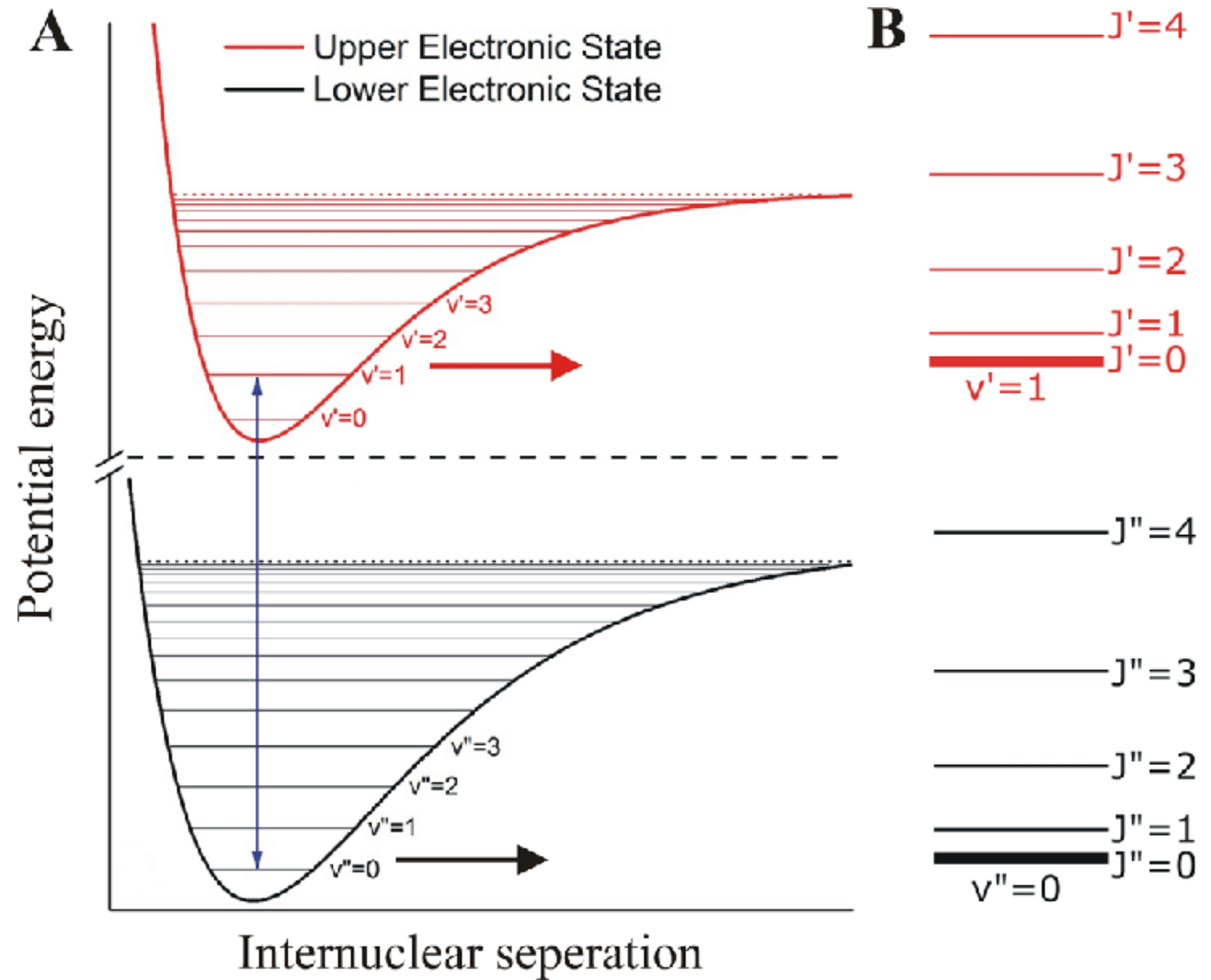
(Nuclear wave equation) $\hat{H}_N(\vec{R})\psi_N(\vec{R}) = E\psi_N(\vec{R})$

(Nuclear Hamiltonian) $\hat{H}_N(\vec{R}) = \hat{T}_N + E_e(\vec{R}) = \frac{\nabla_R^2}{2\mu} + E_e(\vec{R})$

Central force problem!

Energy Levels of a Molecule

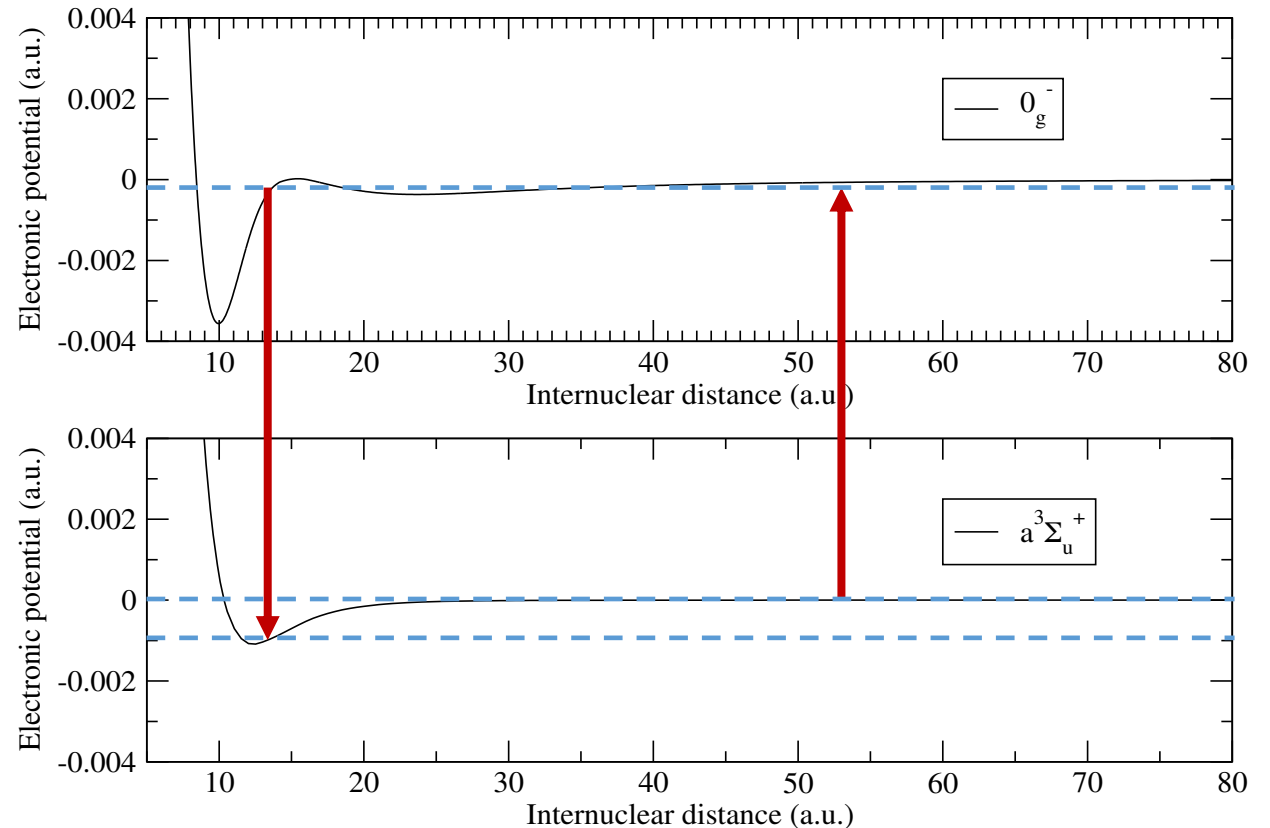
- For a given electronic state (potential), there would be a collection of corresponding vibrational states v and rotational states l (spherical harmonics).
- Our goal is to produce ultracold molecules in their absolute ground state. Difficult to achieve by direct cooling method.



Harilal, S. & Brumfield, Brian & LaHaye, N. & Hartig, K.C. & Phillips, M.. (2018). Optical spectroscopy of laser-produced plasmas for standoff isotopic analysis. Applied Physics Reviews. 5. 021301. 10.1063/1.5016053.

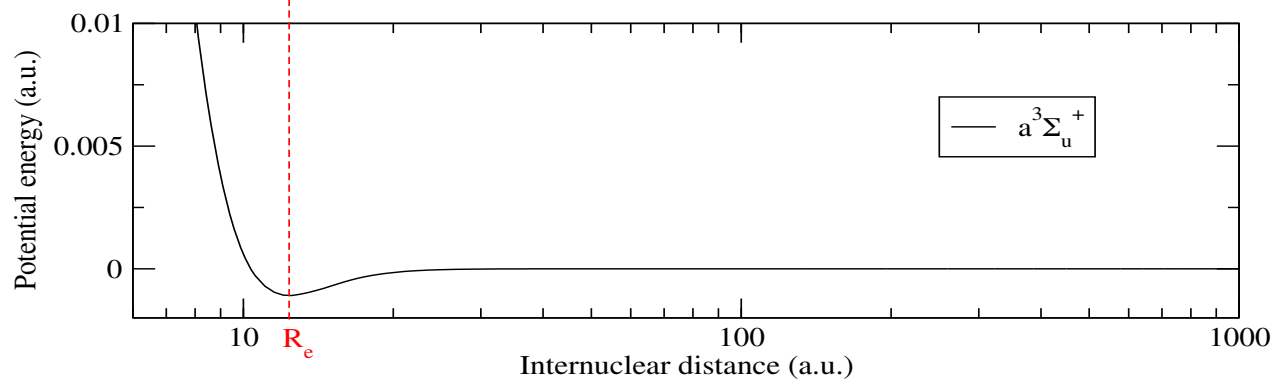
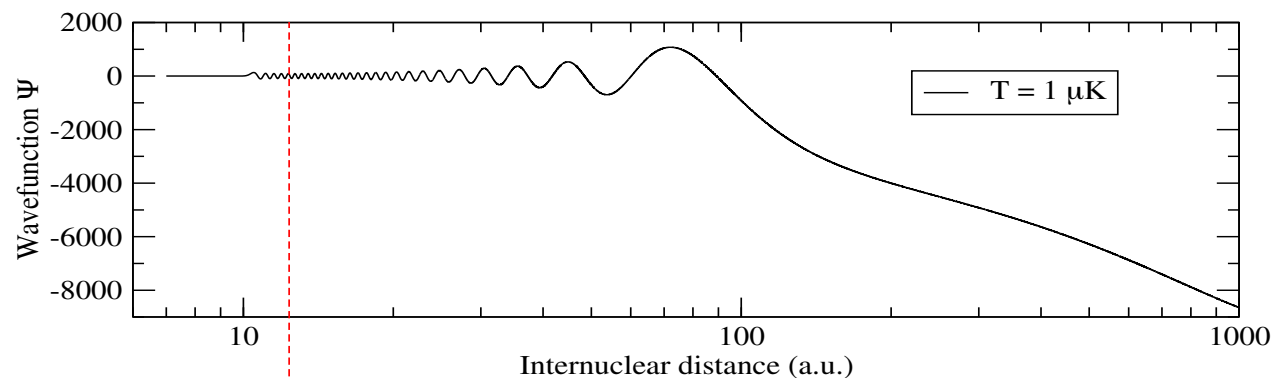
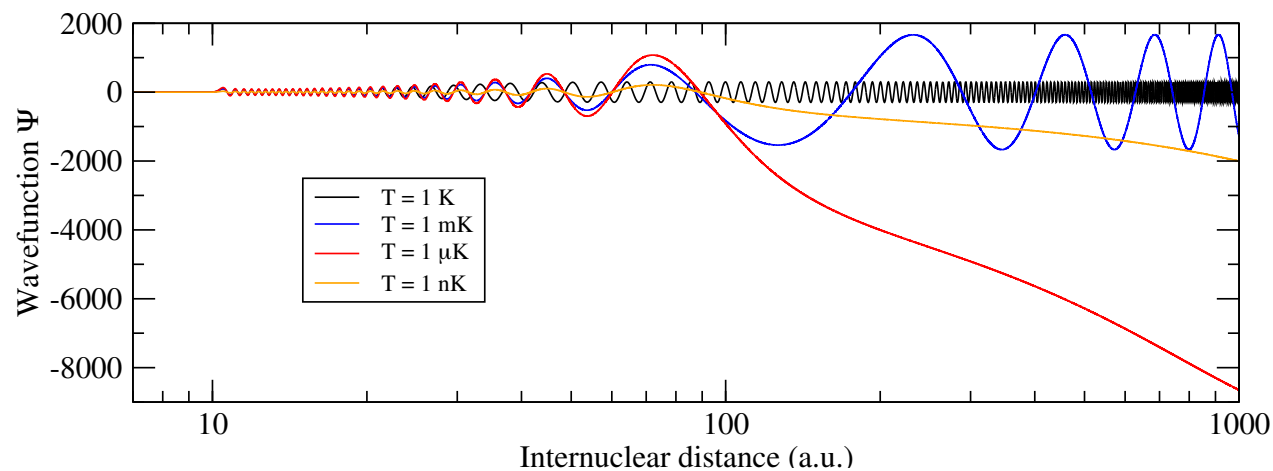
Formation of Ultracold Cs₂ by Photo-association

- The idea is to form the cold molecule by combining two cold atoms with lasers. Two atoms are excited from the continuum of the ground electronic state to an excited electronic bound state forming an excited molecule with high probability of decaying into its ground state. This method was first proven successful by A. Fioretti et al. at Laboratoire Aimé Cotton.

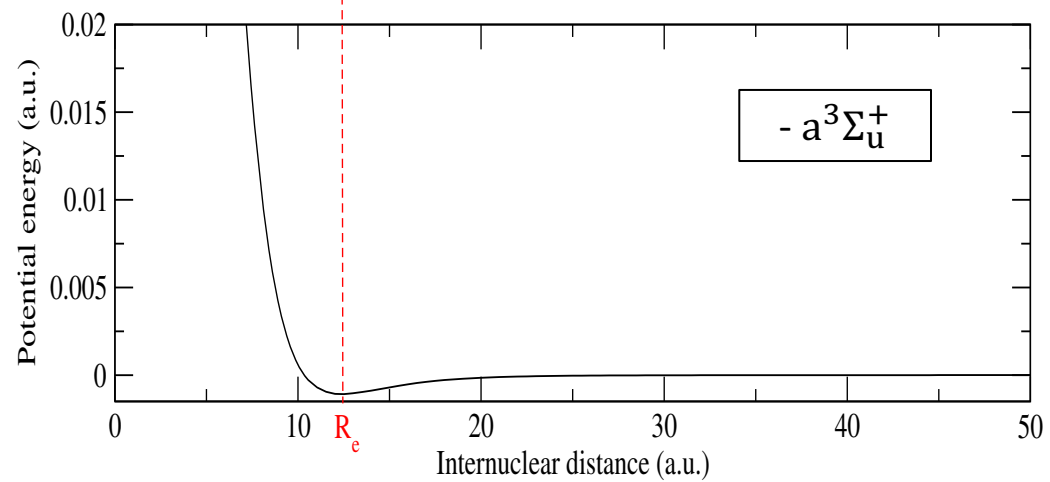
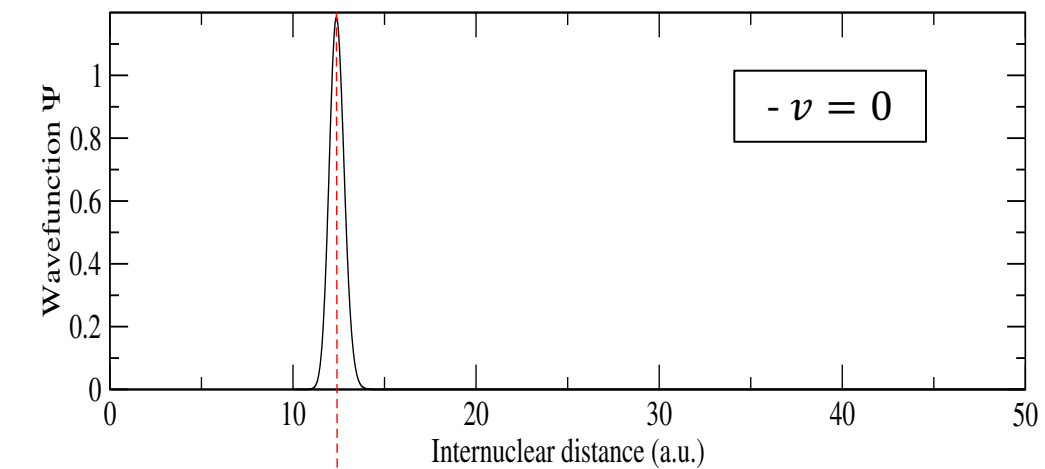


The Continuum Wavefunction

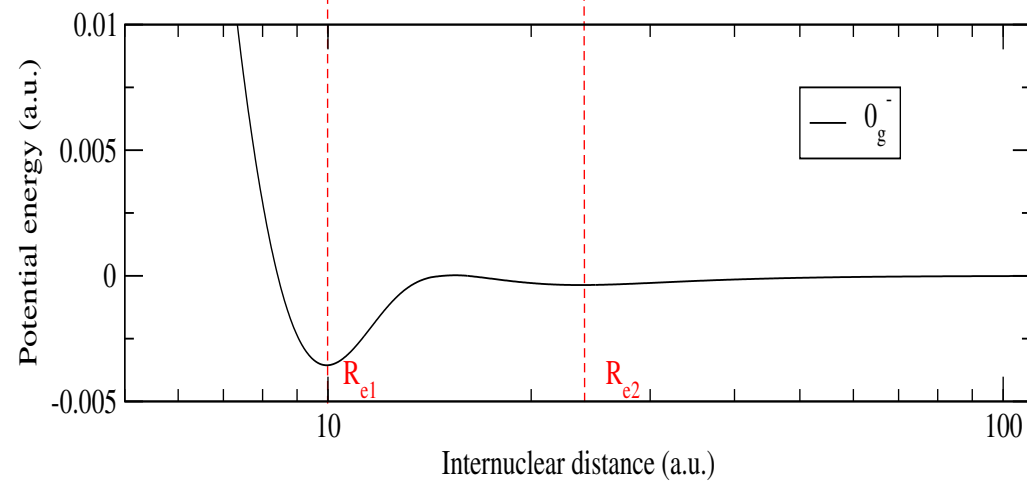
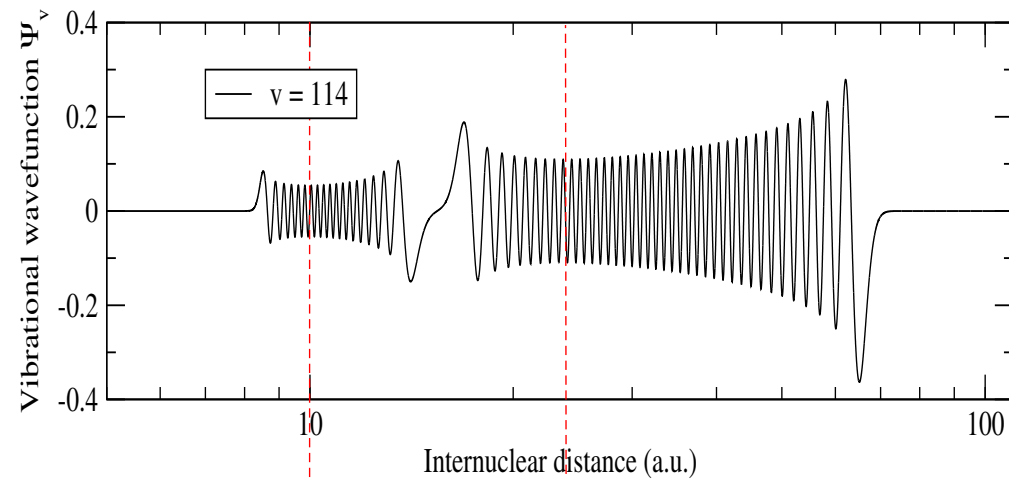
- When the two atoms have energy higher than the dissociation limit, they would be in the continuum state where they become unbound. The wavelength of the wavefunction increases as the potential well gets shallower. The wavefunction will be a plane wave at large distance.



Bound ground state Wavefunctions



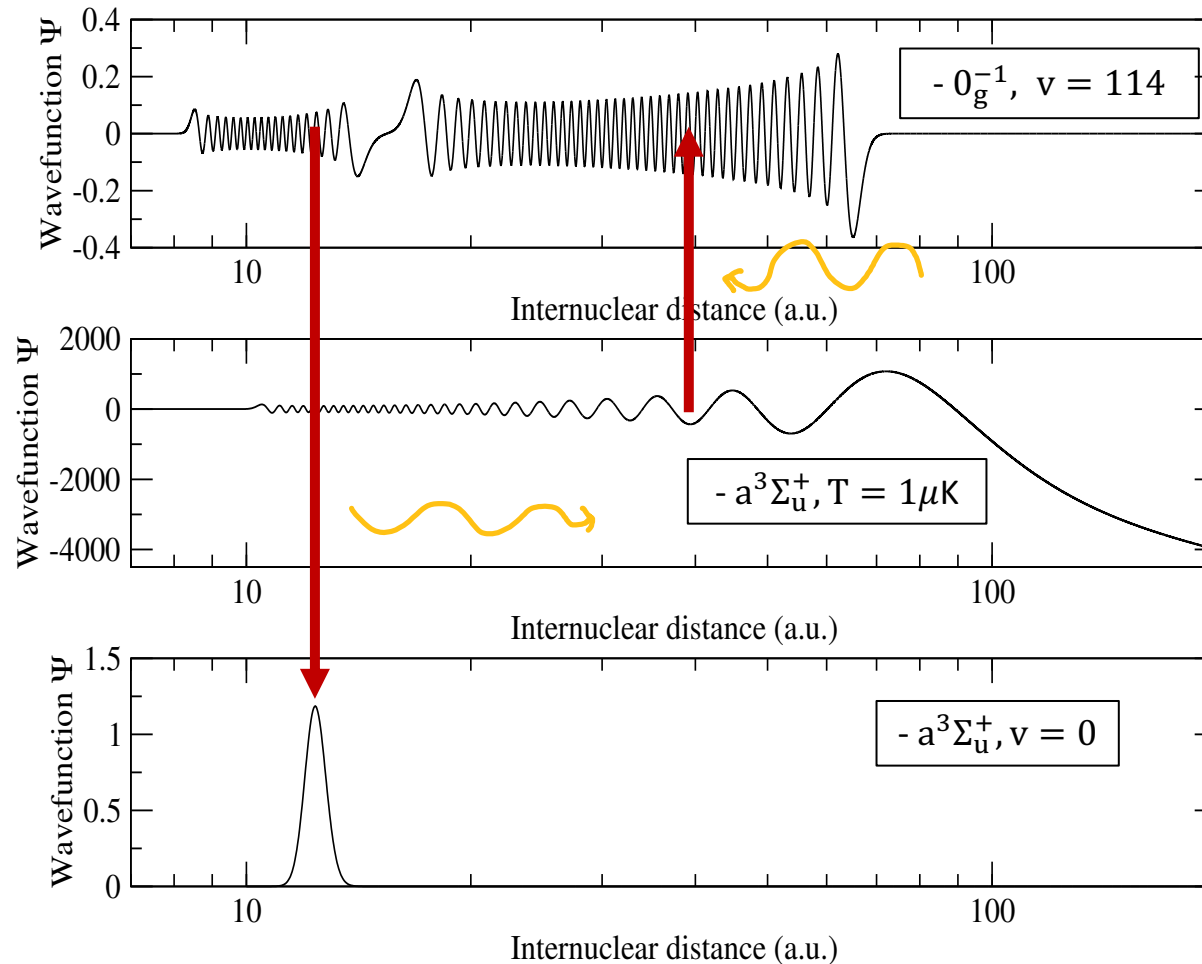
Bound excited state Wavefunctions



A brief sketch of the photoassociation process

Frank-Condon principle:

The probability of the transition between two states is proportional to the overlap of the respective initial and final wavefunctions.



Molecule formed here!

Applications

- Precision measurements: EDM, variation of fundamental constants.
- Quantum simulation: The Hamiltonian of a simulator system can be imitated by taking advantage of the permanent dipoles of the ultracold molecules.
- Controlled chemistry: Well-defined initial states and known state-to-state transition probabilities. This probabilities can be manipulated by different means, e.g. EM fields.