Progress of CR modeling for molecules relevant to fusion

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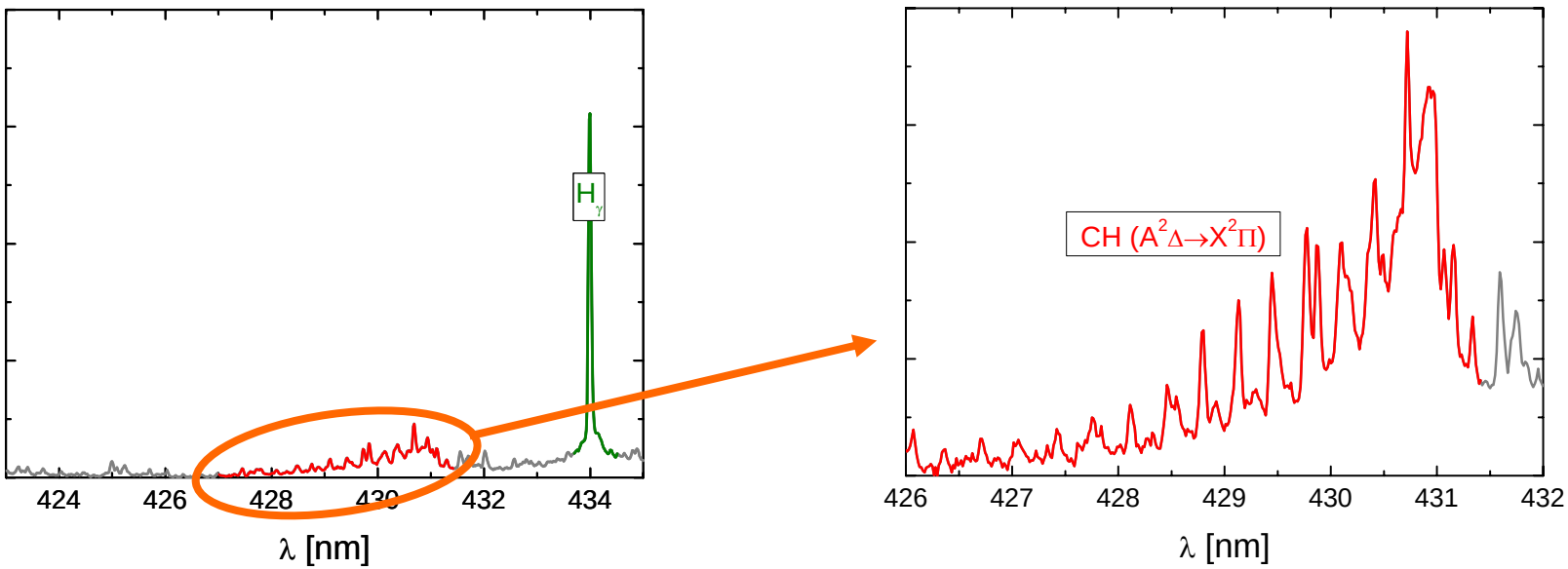
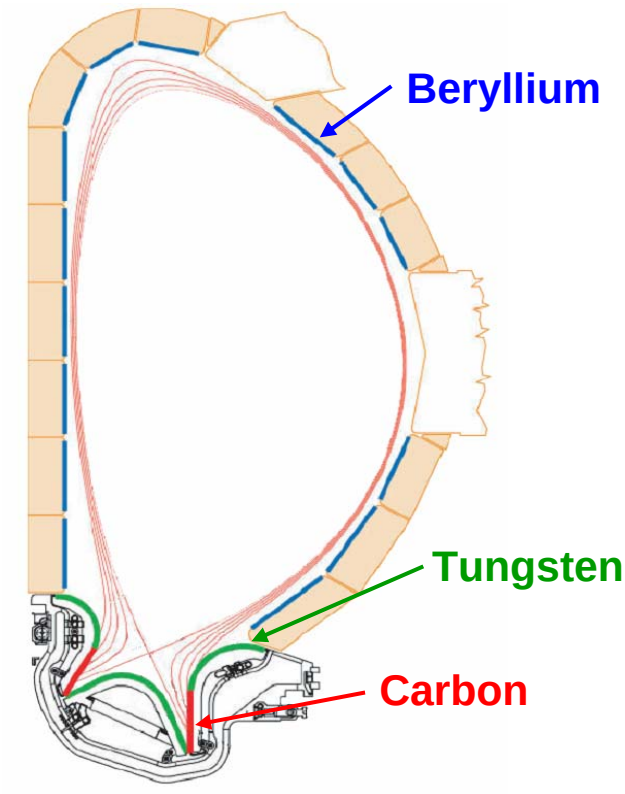


Molecules in fusion experiments



Wall materials

- ITER: Be, W and C
- ASDEX Upgrade: W
- ITER like wall of JET: Be, W
- Boronization of the walls (impurities, recycling)

Low temperatures in the plasma edge
⇒ formation of molecules

Recycling at the wall

H_2, D_2, T_2, HD, HT, DT

Plasma wall interaction

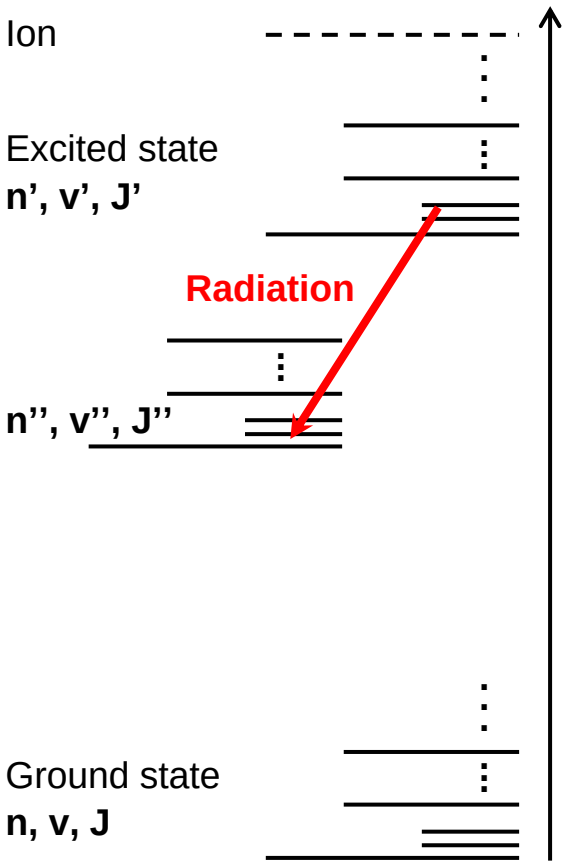
CH, CD, CT, C_2

BeH, BeD, BeT

BH, BD, BT

CR models for molecules

Split-up of electronic energy levels due to vibrational and rotational excitation



$$\varepsilon = n_{v'}^{n'}(J') \cdot A_{v'v''}^{n'n''}(J', J'')$$

CR models for molecules
much more complex than for atoms

Vibrationally and rotationally resolved cross sections and transition probabilities

- Coupling with molecules, atoms or ions (e.g. dissociative excitation or recombination)
- Isotope effect
- Low intensity of single lines ⇒ no relevance of optical thickness
- Thermalization ⇒ Rotational levels neglected in most CR models

Potential curves of H_2

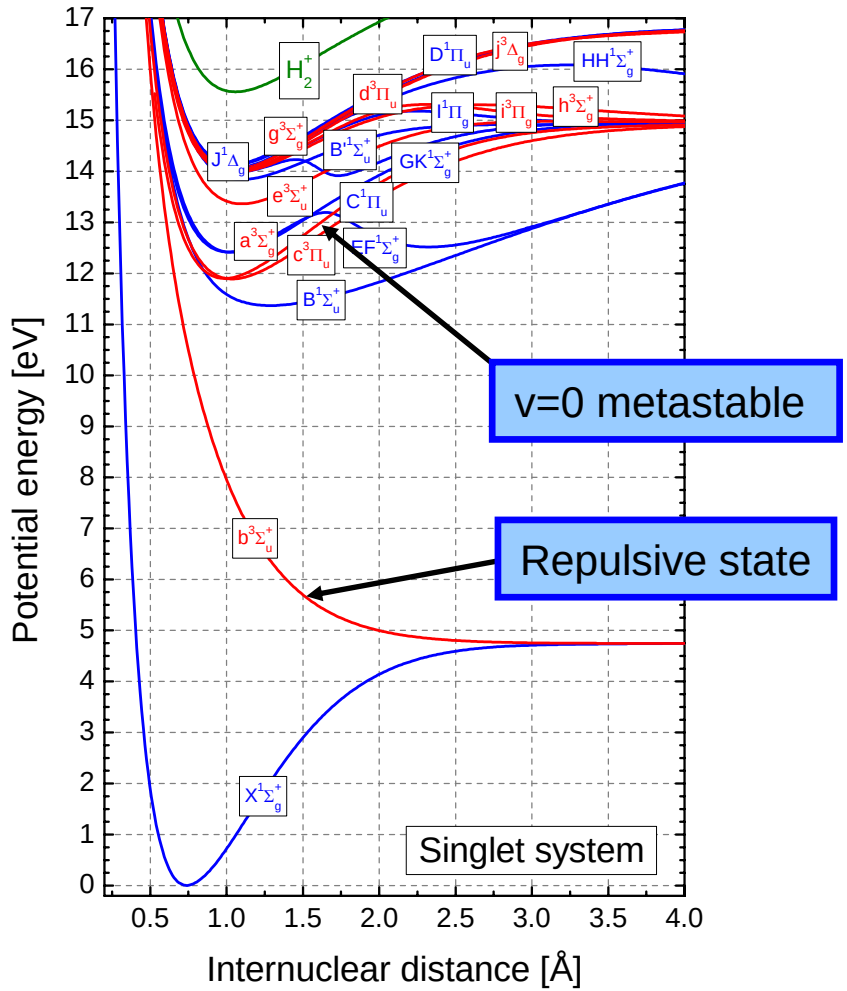
Born-Oppenheimer approximation

Electronic and nuclear motion can be separated due to mass ratio

⇒ Separate treatment of electronic, vibrational (and rotational) excitation

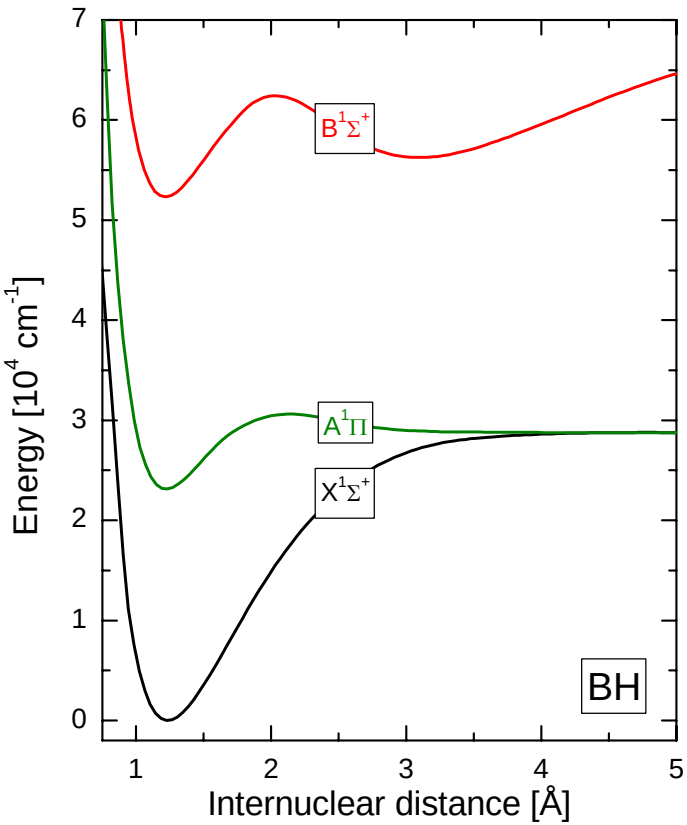
$$\Phi(\mathbf{R},\mathbf{r}) = \Upsilon(\mathbf{R},\mathbf{r}) \cdot \Psi(\mathbf{R})$$

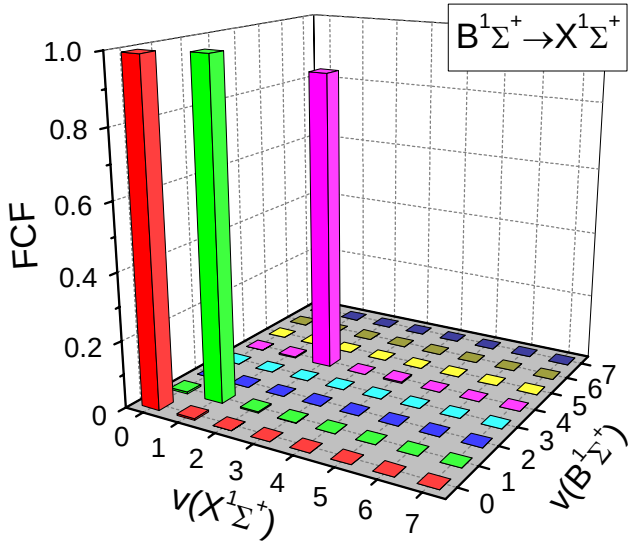
Potential curves: eigenvalues of electronic wave functions

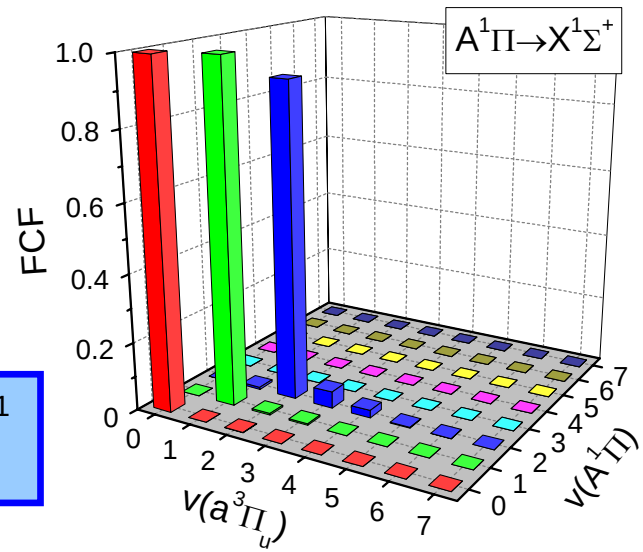


TraDiMo for BH

$$FCF = \left|\langle \Psi | \Psi' \rangle\right|^2$$



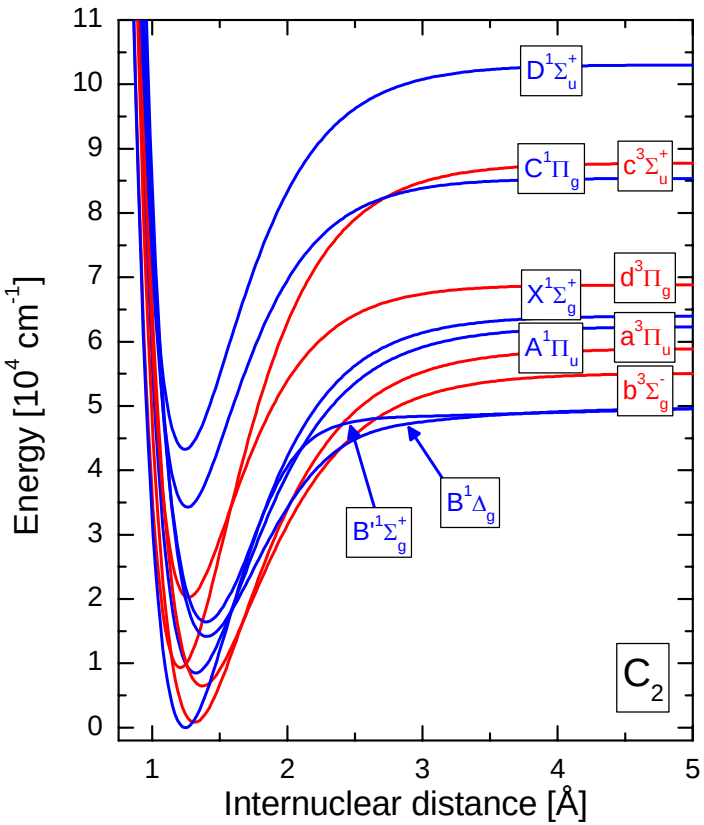


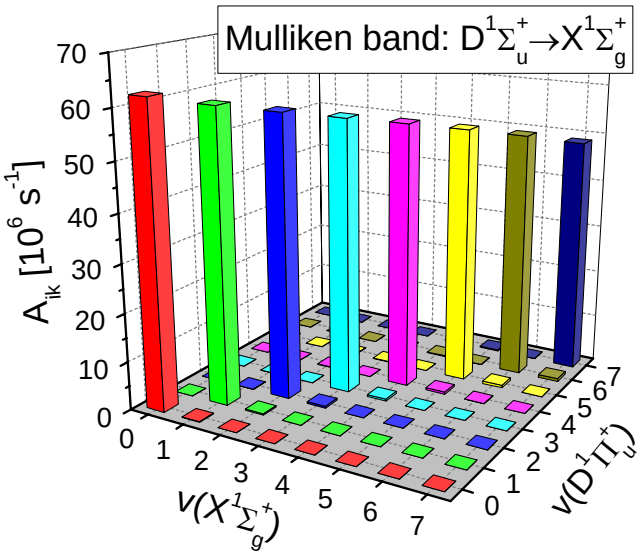


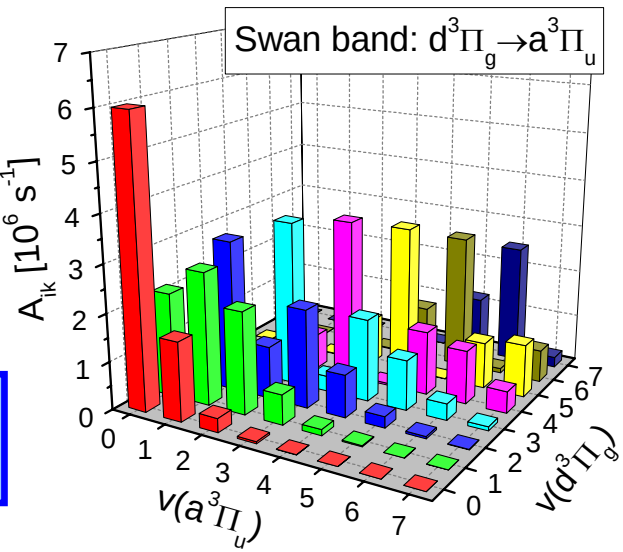
Potential curve of B^1 state: double well

TraDiMo for C_2

$$A_{v'v''} \propto \left| \langle \Psi' | M_{el} | \Psi'' \rangle \right|^2$$

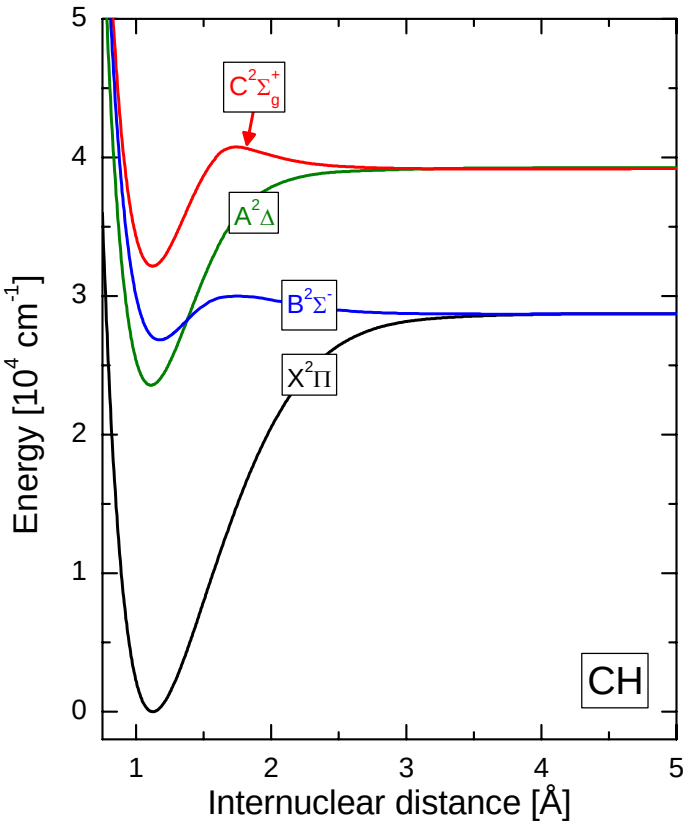




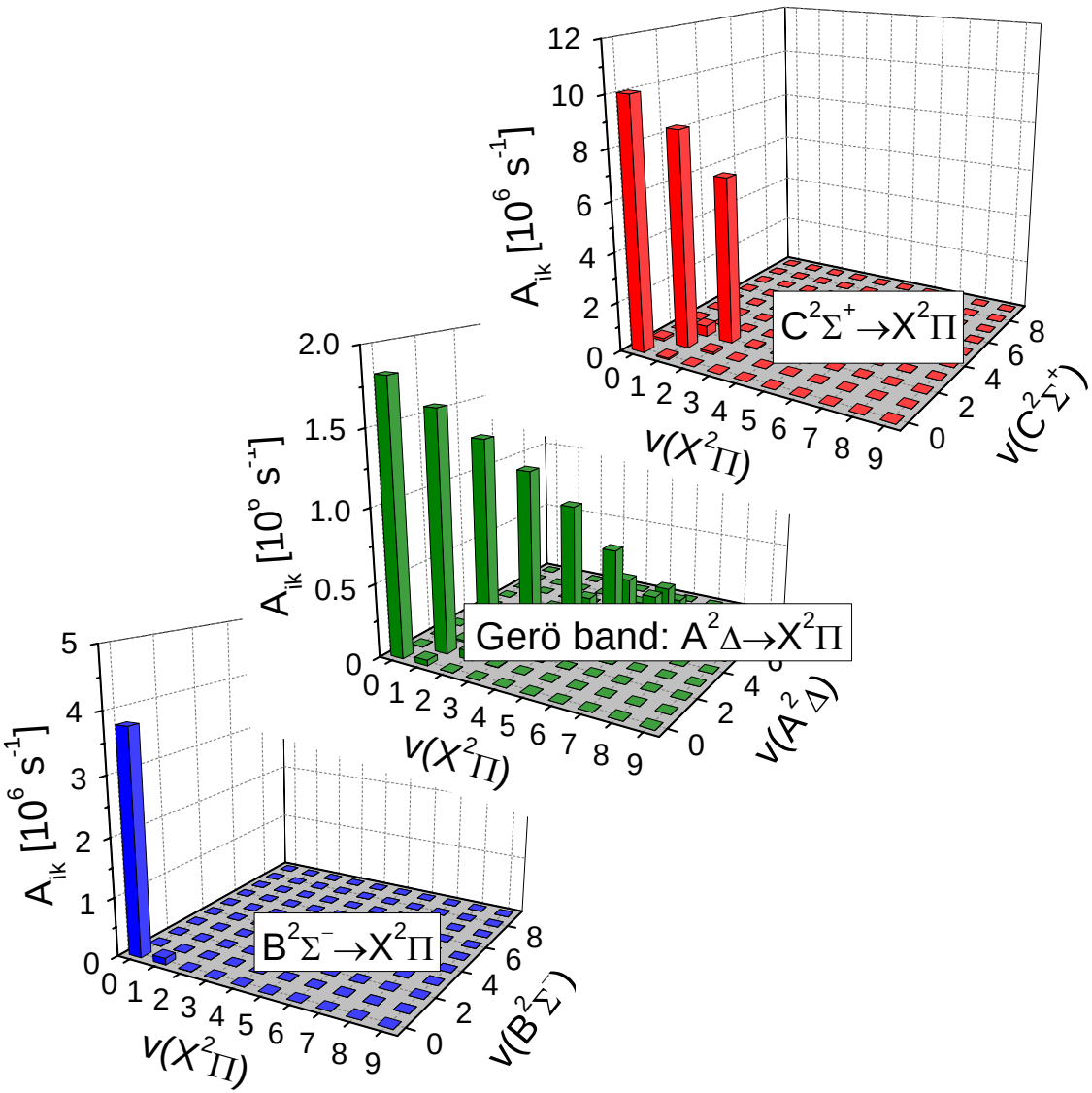


Singlet system and triplet sytem

TraDiMo for CH



Different shape of potential curves

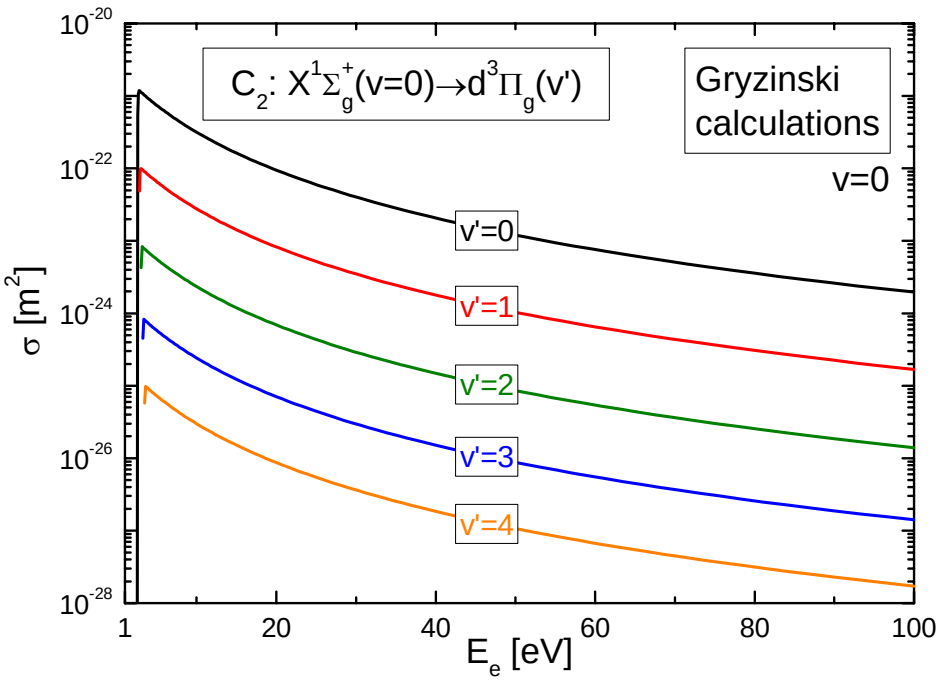


Excitation rate coefficients: forbidden transitions

Gryzinski method

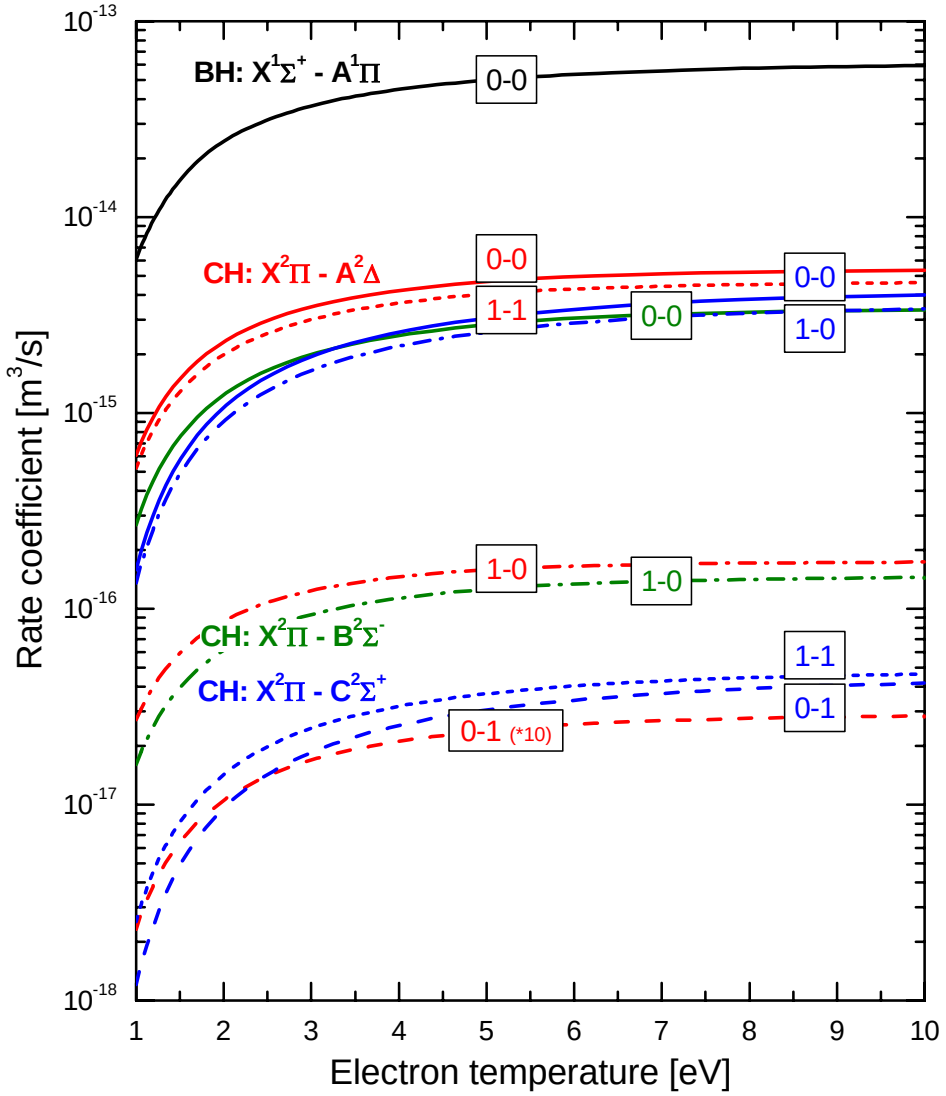
Based on Franck Condon Factors, low accuracy

- In principle very simple method
- Some obscurities, like definition of “next allowed level” (difficult in molecules)
- Calculations for H_2, C_2, CH



More accurate data for forbidden transitions highly desirable

Excitation rate coefficients: allowed transitions



Impact parameter method

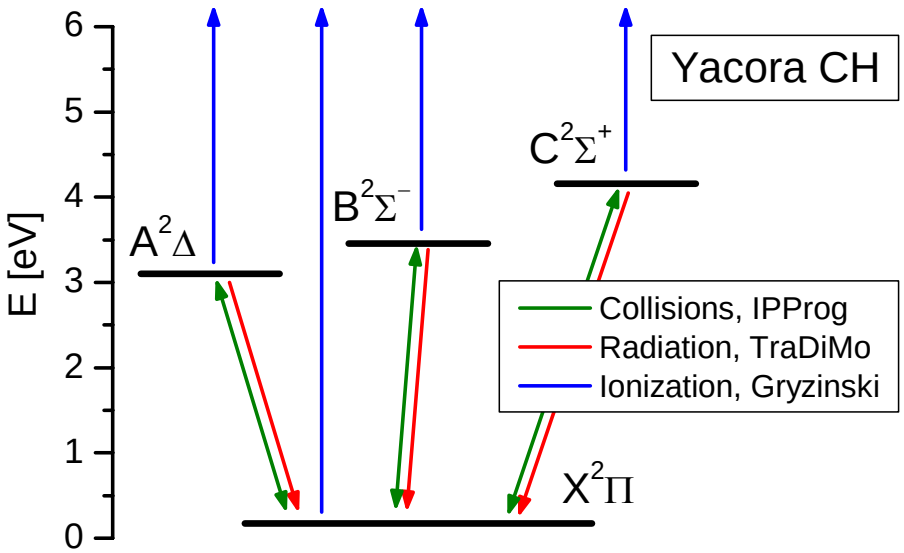
Based on transition probabilities, very accurate

- IPProg: simple tool to calculate rate coefficients
- Good agreement with Born-Bethe calculations*
- Calculations for H_2, C_2, CH, BH

Sufficient data basis for allowed transitions

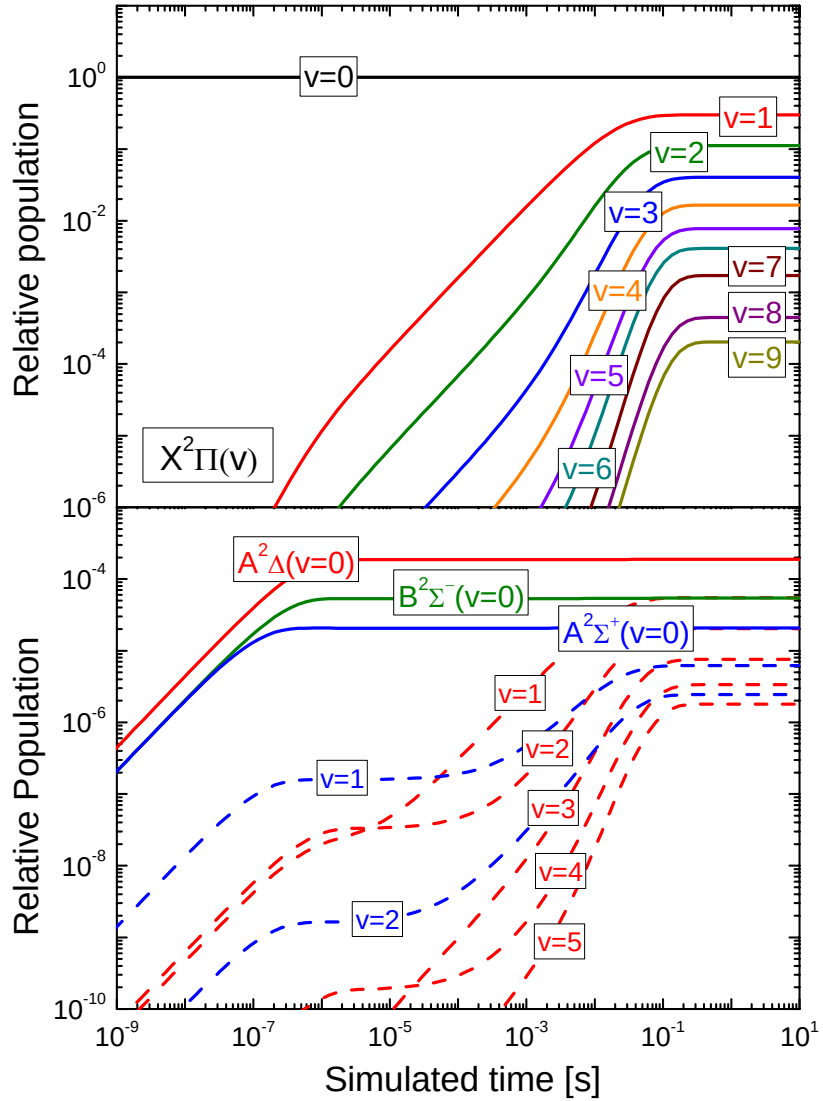
*: R. Celiberto et al, Plasma Phys. Control. Fusion 51, 2009, 085012

Yacora: CR model for CH

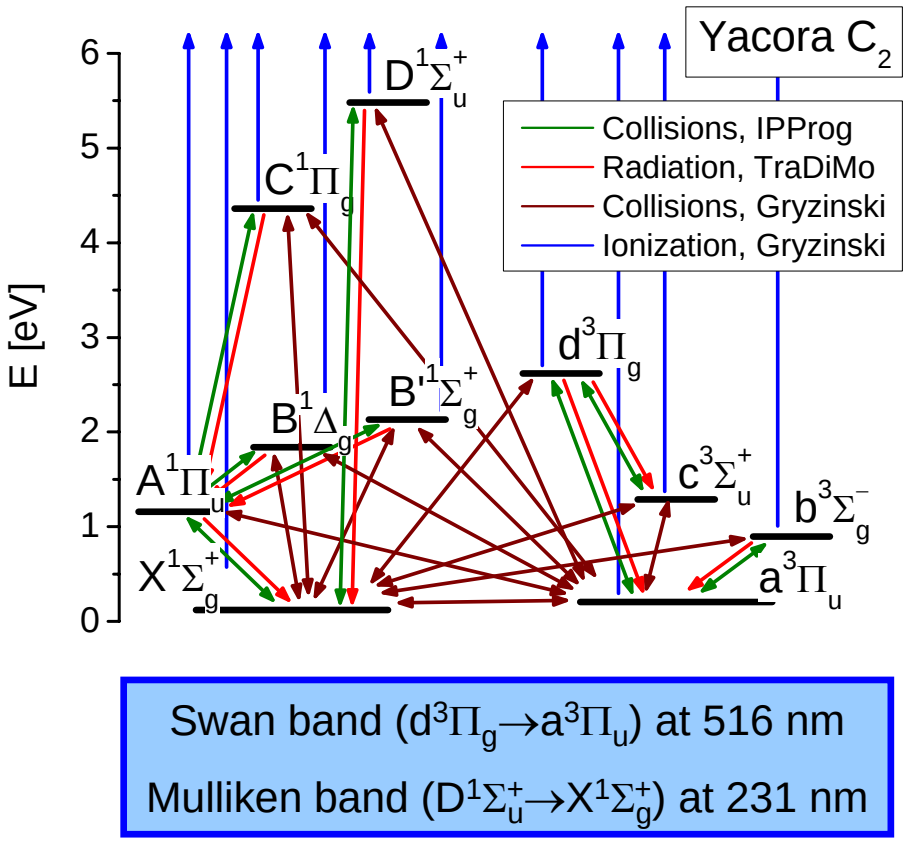


Gerö band ($A^2\Delta \rightarrow X^2\Pi$) at 431 nm

- Temporal evolution of population densities
- Different typical time scales, interplay of electronic and vibrational population



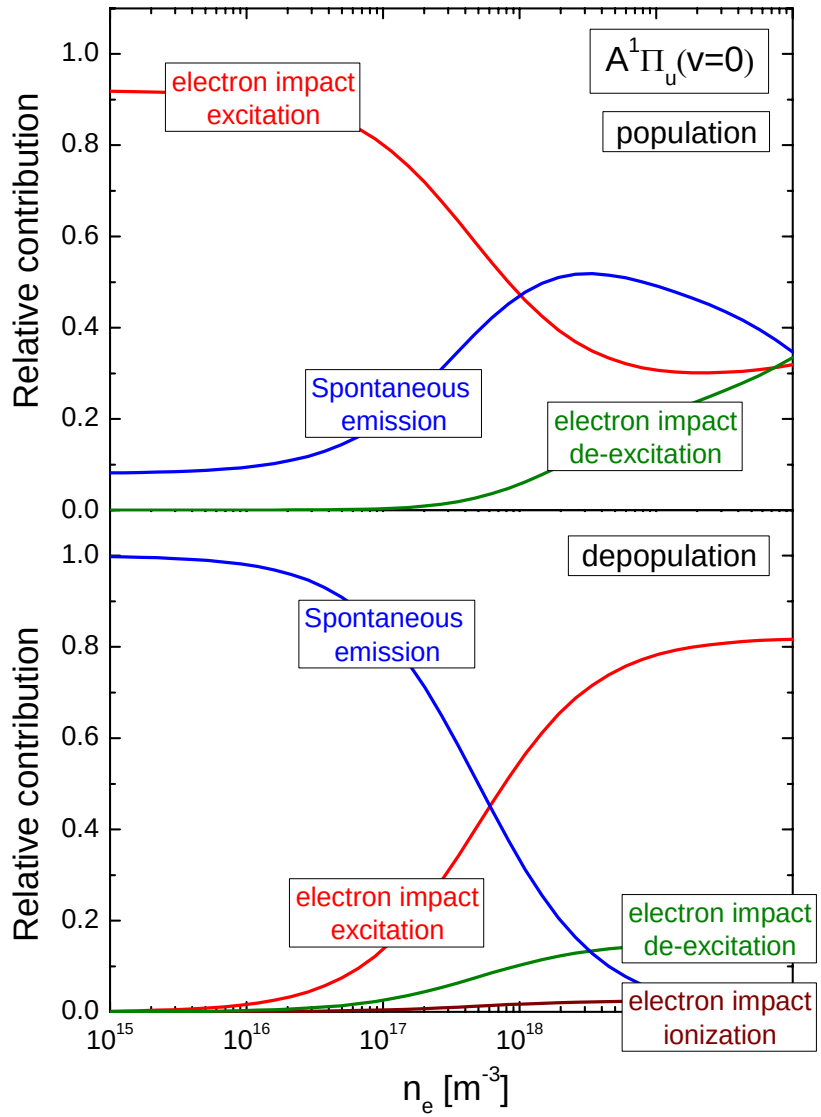
Yacora: CR model for C_2



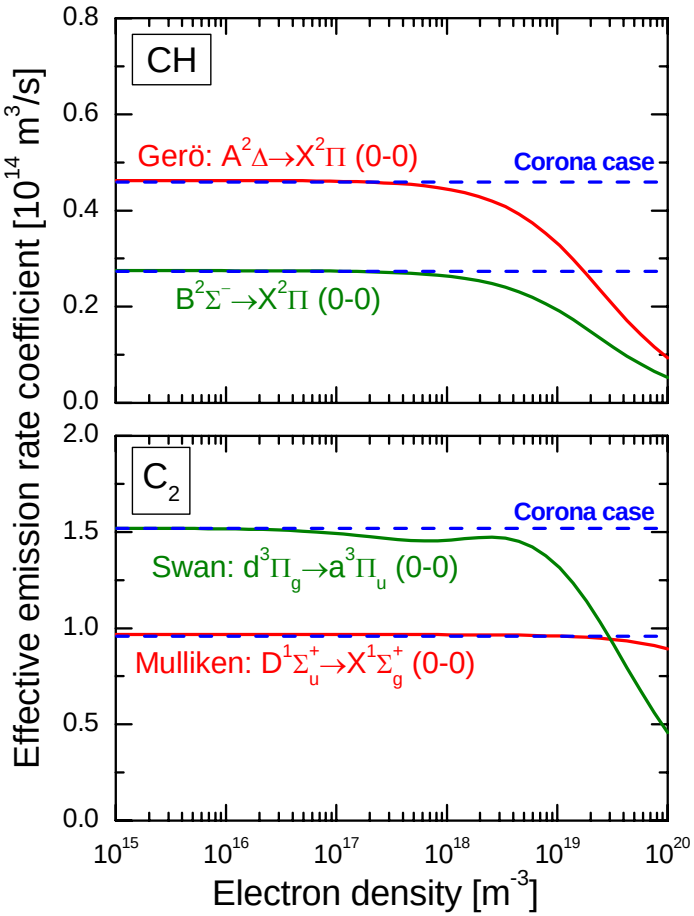
Swan band ($d^3\Pi_g \rightarrow a^3\Pi_u$) at 516 nm

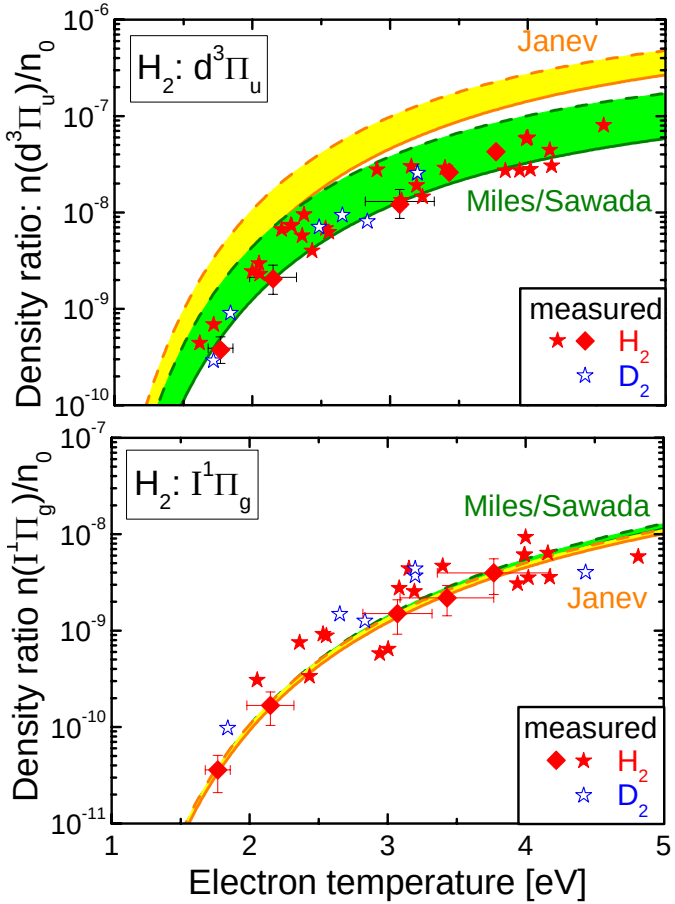
Mulliken band ($D^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$) at 231 nm

- Strong influence of plasma parameters on relevance of excitation and de-excitation processes



Application of CR models: effective rate coefficients





CH/C_2: Deviation from corona model in a wide parameter range, application of the CR model mandatory

H_2: drastically improved agreement of measured and calculated population densities by exchange of input data

Overview and conclusions

Potential curves *Literature*	H_2	C_2, CH, BH, BeH
FCF, Transition probabilities *TraDiMo*	H_2, D_2, T_2, HD, DT	C_2, CH, CD, CT, BH, BeH
Electron impact cross sections *IPProg, Gryzinski method*	H_2 *(some transitions)*	C_2, CH, BH, BeH
CR model *Yacora*	H_2	C_2, CH

- Proved set of codes for generating input data and CR models
- Foundation for CR modeling of fusion relevant diatomic molecules
- Additional effort necessary (e.g. replace Gryzinski cross sections)