Molecular Data and ADAS.

Francisco Guzmán The ADAS Team

ADAS-EU
University of Strathclyde

ADAS WORKSHOP – October 2009

Outline

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Objetives

1. Extend ADAS Database to molecular data

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2. Provide Molecular data tools to use in plasma edge and divertor calculations and experiments.

Format: Molecular Indexes

indx_s Different molecular and atomic species.

indx_p Different process departing from a specie.

indx_e Different electronic states of each specie.

indx_v Vibronic index for each electronic state.

indx_r (internal) Reactions from one electronic state of one specie to another different specie or/and electronic state.

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Pre format file

```
H_2      / electron impact                                              adf50

species
-------
 ind_s   identity   e-config  e-coupling   classif    ch_ion   bwno_i   ch_dis  bwno_d
 -----   --------   --------  ----------   -------    ------   ------   ------  ------
   1     H_2        dia-ua    dia-term     vibro      1->2      1090.   1->4+4  234.
                                                                        1->5+6  112.
   2     H_2^+      dia-ua    dia-term     vibro                        2->4+5
   3     H_2^-      dia-ua    dia-term     vibro                        3->4+6
   4     H          atm       atm-term
   5     H^+        atm
   6     H^-

process
-------

ind_p                              path                                    description
-----  ------------------------------------------------------------   ---------------------
  1    e+H_2(v=0) -> H_2^-(X(2)S(+)(u),B(2)S(+)(u)) -> e + H_2(v')  vib exc via e attach
  2    e+H_2(v=0) -> e + H_2*(1)N                                   vib unr. exc.-> singlet
  3    e+H_2(v=0) -> e + H_2*(3)N                                   vib unr. exc.-> triplet
  4    e+H_2(v) -> e + H_2*(1)N                                     vib unr. exc.-> singlet
  5    e+H_2(v) -> e + H_2*(3)N                                     vib unr. exc.-> triplet
  7    e+H_2(v) -> e + H_2*(1)N -> e + H(1s) + H(nl)                vib unr. diss. exc.-> singlet
  8    e+H_2(v) -> e + H_2*(3)N -> e + H(1s) + H(nl)                vib unr. diss. exc.-> triplet
  9    e+H_2(v) -> e + H_2*(1)N(v')                                 vib res. exc. -> singlet
 10    e+H_2(v) -> e + H_2*(3)N(v')                                 vib res. exc. -> triplet
 11    e+H_2*(N(v)) -> e + H_2*(1)N'(v')                            vib res. exc. -> singlet
 12    e+H_2*(N(v)) -> e + H_2*(3)N'(v')                            vib res. exc. -> triplet
 13    e+H_2(N(v)) -> e + e + H_2+(2)                               vib unr. ion. to ground state
 ...
```

Pre format file

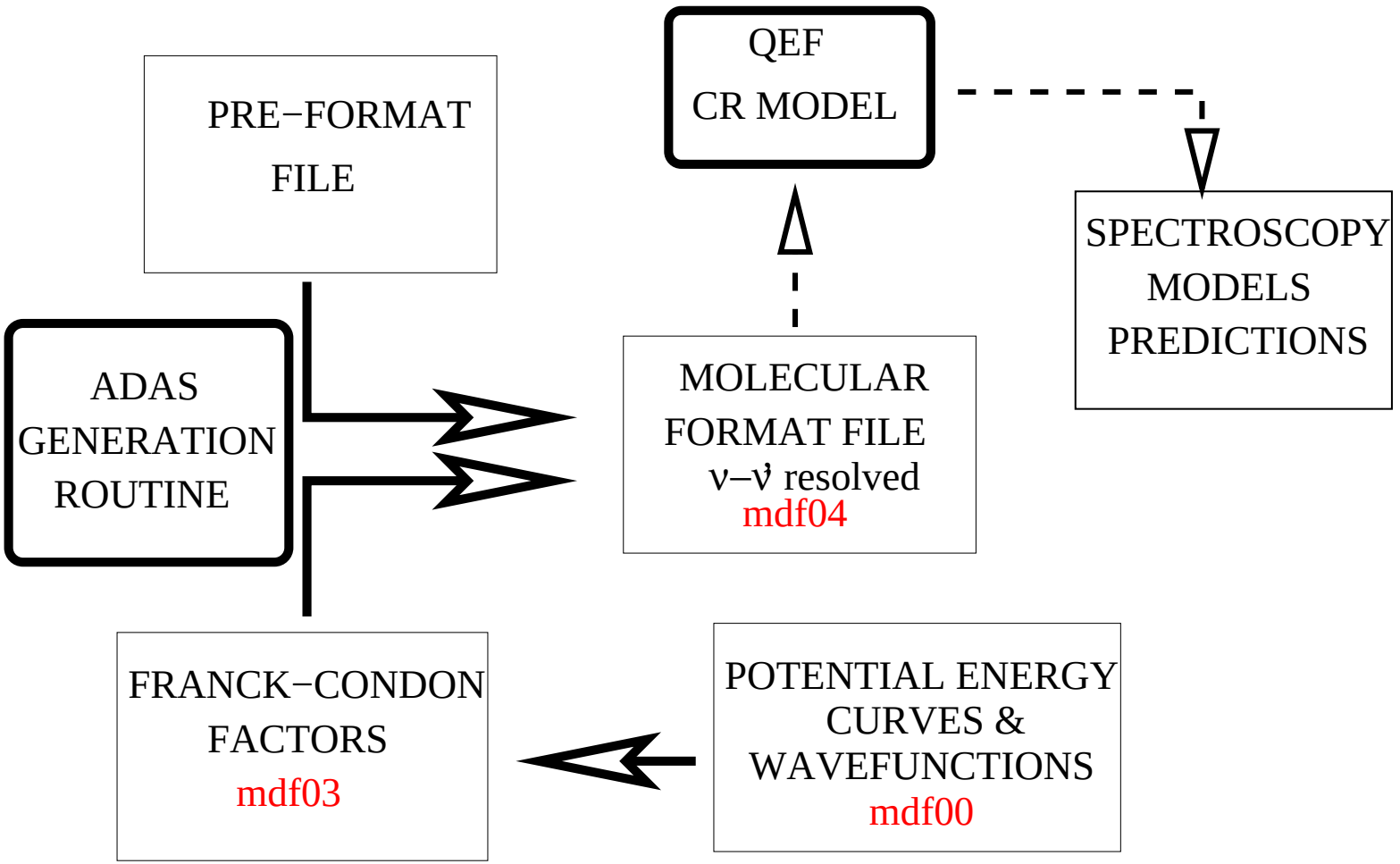
```
states
------
 ind_s   indx_e  e-con-ua  e-con-sa   coupled state   (wt.-1)/2
 -----   ------  --------  --------    -----------    ---------
   1       1     1ssg1ssg    1s1s       (1)S(+)(g)        0.0
   1       2     1ssg2ssg    1s2s       (1)S(+)(g)        0.0
   1       3     1ssg2psu    1s2p       (1)S(+)(u)        0.0
   1       4     1ssg2ppu    1s2p       (1)P( )(u)        1.0
   1       5     1ssg3ssg    1s3d       (1)S(+)(g)        0.0
   1       6     1ssg3psu    1s2s       (1)S(+)(u)        0.0
   1       7     1ssg3ppu    1s3d       (1)P( )(u)        1.0
   1       8     1ssg3dsg    1s2p       (1)S(+)(g)        0.0
   1       9     1ssg3dpg    1s3d       (1)P( )(g)        1.0
   1      10     1ssg3ddg    1s3d       (1)D( )(g)        2.0
   1      11     1ssg4ssg    1s3p       (1)S(+)(g)        0.0
   1      12     1ssg4psu    1s3s       (1)S(+)(u)        0.0
   1      13     1ssg4ppu    1s4p       (1)P( )(u)        1.0
   1      14     1ssg4dsg    1s3d       (1)S(+)(g)        0.0
   ...
```

Pre format data

- The boolean variable *numer* indicates if numerical data are available (1) or not (0).
- Numerical values will be filled while the formula index *form* (form=0 -> no formula provided) will give the fitting formula in which the parameters *par_val* are used.

```
ch_in              ind_p         ch_out       ch_dis
-----             ------         ------       ------
s   e     v                    s   e   v
1   1     0         1          1   1   1
                    parameters & values
                    -------------------
categ=1  tcode=3  a_val= 0.00e+00  a_dis= 0.00e+00  form=1 par=1 numer=1  DE=   0.516e+00
     te=   2.00e+00  3.00e+00  4.00e+00  5.00e+00  6.00e+00  7.00e+00  8.00e+00
           2.00e+01  3.00e+01  4.00e+01  5.00e+01  6.00e+01  7.00e+01  8.00e+01
           2.00e+02  3.00e+02  4.00e+02  5.00e+02  6.00e+02  7.00e+02  8.00e+02
    omg=   2.00e+00  3.00e+00  4.00e+00  5.00e+00  6.00e+00  7.00e+00  8.00e+00
           2.00e+01  3.00e+01  4.00e+01  5.00e+01  6.00e+01  7.00e+01  8.00e+01
           2.00e+02  3.00e+02  4.00e+02  5.00e+02  6.00e+02  7.00e+02  8.00e+02
par_val=   1.00e+00
```

Generation of Molecular files



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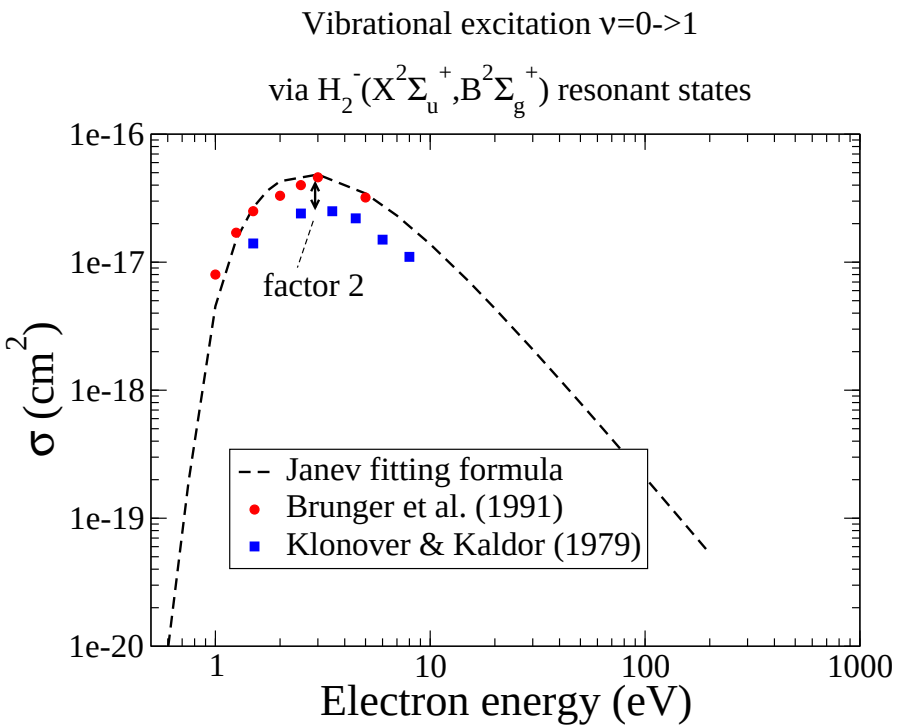
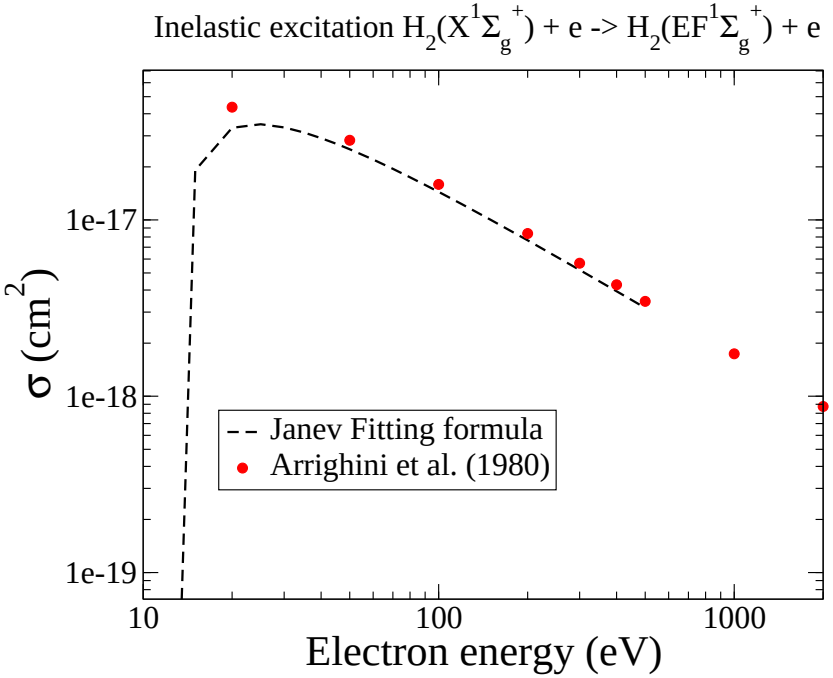
- Franck Condon Factors are needed. Current set provided by D. Wünderlich[1].

[1] ADNDT **92**, 853 (2006)

Fitting vs. numerical data

The fitting formula try to get a continous behauviour from the numerical data choosing the most reliable sets of data in each energy range and each process.





To do and current work

- Cross-check fitting formulas and numerical data.
- Create final files and the generation subroutines.
- Create a population Model
- Generate Coefficient rates from cross sections.
- Extend to other System (Homonuclear: N_2, Heteronuclear: BeH (?)).

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Calling for Data: All molecular (H_2) relevant data are welcome.

THANK YOU