# Data Needs and Modeling of the Upper Atmosphere

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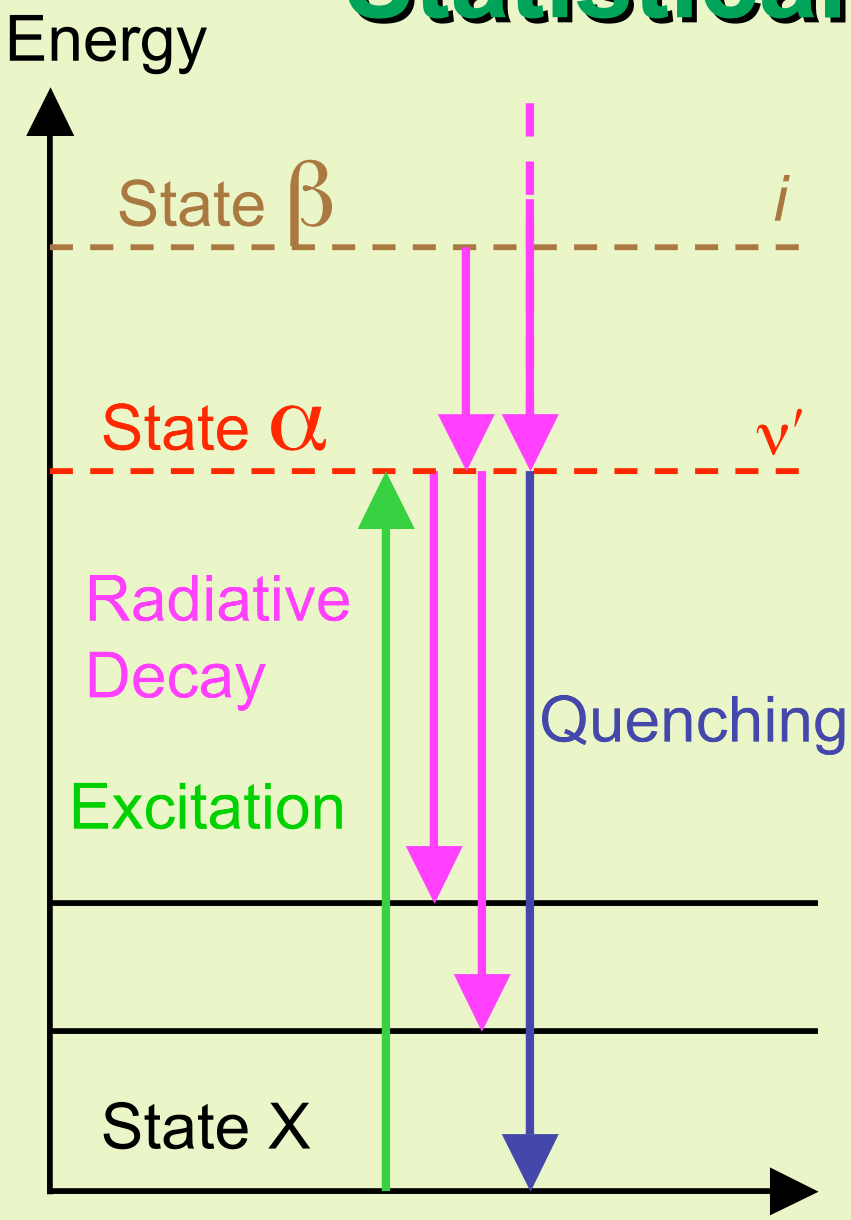
# Introduction

- We aim to investigate:
  - Importance of electron driven processes in atmospheric modeling.
  - Importance of using more accurate experimental and theoretical data,
    - particularly electron-impact excitation cross sections, although all data inputs are crucial in this respect (see later).

# Statistical equilibrium



Statistical equilibrium - solve simultaneous continuity equations until:
population($\alpha_{\nu'}$) x loss rate = total gain of $\alpha_{\nu'}$

$$k^{\alpha}_{\nu'0}\, n^{\mathrm{X}}_{0} + \sum_{\beta}\sum_{i} A^{\beta\alpha}_{i\nu'}\, n^{\beta}_{i} = \sum_{i,j,k}\left(A^{\alpha j}_{\nu' i} + Q^{\alpha k}_{\nu'}\right) n^{\alpha}_{\nu'}$$

# Photochemical model

- Photoionisation, photodissociation

$O + h\nu \rightarrow O^+(^4S), + e^-$

(also $O^+(^2D)$, $O^+(^2P)$ )

$O_2 + h\nu \rightarrow O_2^+ + e^-$

$N_2 + h\nu \rightarrow N_2^+ + e^-$

$NO + h\nu \rightarrow NO^+ + e^-$

$N(^4S) + h\nu \rightarrow N^+ + e^-$

$N_2 + h\nu \rightarrow N(^4S) + N^+ + e^-$

$O_2 + h\nu \rightarrow O + O^+ + e^-$

$NO + h\nu \rightarrow O + N(^4S)$

$N_2 + h\nu \rightarrow N(^2D) + N(^4S)$

- Atmospheric chemistry (partial list)

$N(^2D) + O_2 \rightarrow NO^* + O$

$N(^4S) + O_2 \rightarrow NO + O$

$NO + N(^4S) \rightarrow N_2 + O$

$NO + O_2^+ \rightarrow NO^+ + O_2$

$NO + N(^2D) \rightarrow N_2 + O$

$NO^+ + e^- \rightarrow N(^2D) + O$

$N_2^+ + O \rightarrow N(^2D) + NO^+$

$N(^2D) + O \rightarrow N(^4S) + O$

$NO^+ + e^- \rightarrow N(^4S) + O$

$N_2^+ + O_2 \rightarrow O_2^+ + N_2$

# Model improvements

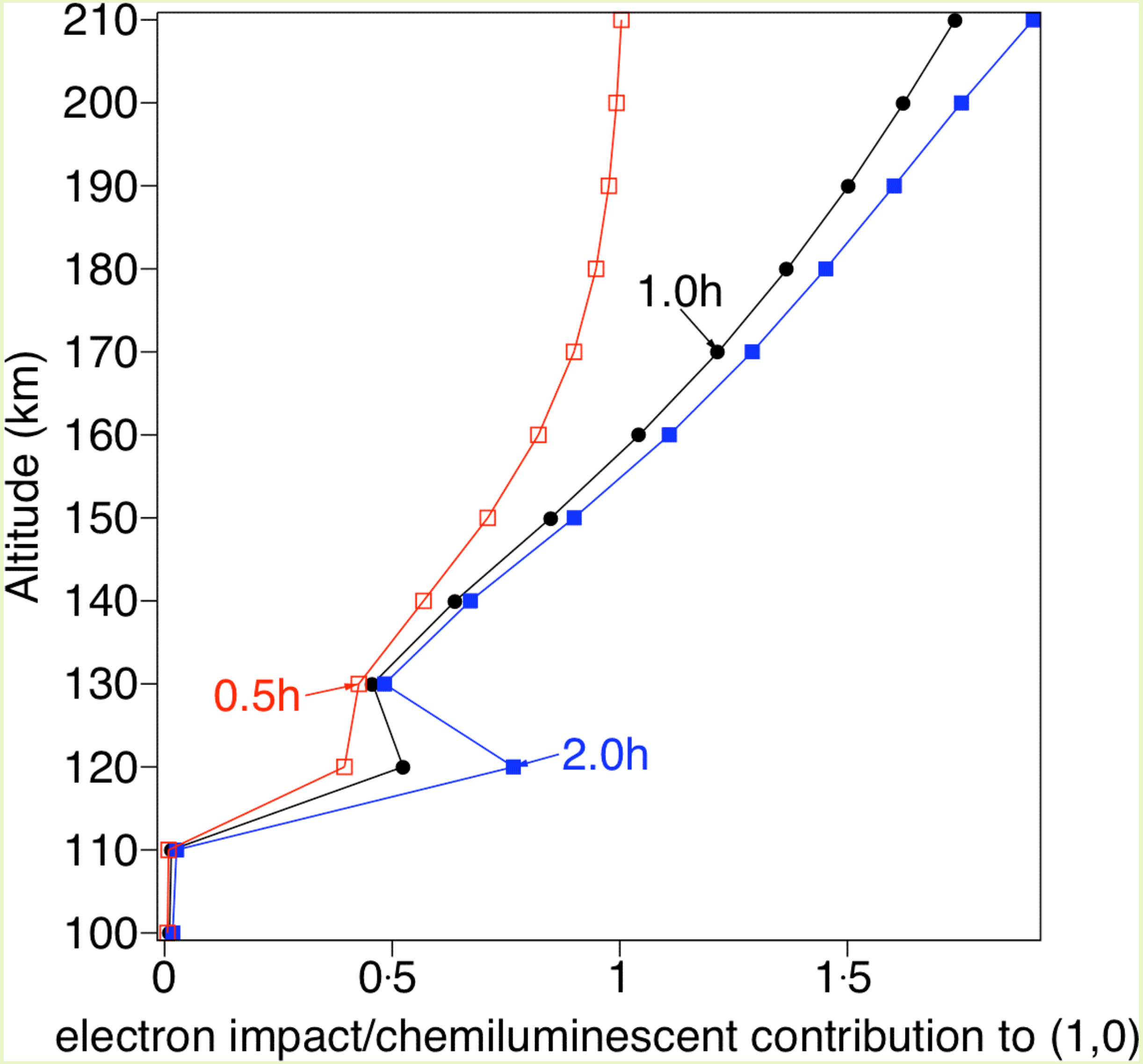
- We have incorporated new features over the basic statistical equilibrium approach to model atmospheric behaviour. These include:
  - Photochemical model
    - Necessary to predict electron density, NO production.
  - Ambipolar and molecular diffusion
    - Important above 200 km.
  - Time-step calculation
    - Required for aurora when equilibrium is not reached.
  - Statistical equilibrium plus time-step calculations
    - Required to merge fast excitation-deexcitation processes into time-step calculation of electron density.

# New results:Investigating the origin of IR emission in NO*

- Auroral (1,0) emission from vibrationally excited NO has been assumed to be due to the chemiluminescent reaction
  - $N(^2D) + O_2 \rightarrow NO^*(v'=1–12) + O$
- We are investigating the contribution of electron scattering to auroral NO emission, based on the new electron impact cross sections for NO measured at Belgrade and the ANU.
- This requires detailed atmospheric modeling, as the ratio of electron impact to chemiluminescent contributions depends on atmospheric parameters, including:
  - Thermal electron temperature (increased by the aurora).
  - Quenching rates in collisions with $N_2$, $O_2$ and O.
  - NO and $N(^2D)$ densities.

# New results involving IR emission in NO*

- Calculated ratio of contributions of electron-impact excitation and chemiluminescent production to the (1,0) infrared emission from NO in an IBC II$^+$ aurora after:
  - ☐ 0.5 hours
  - ● 1.0 hour
  - ■ 2.0 hours



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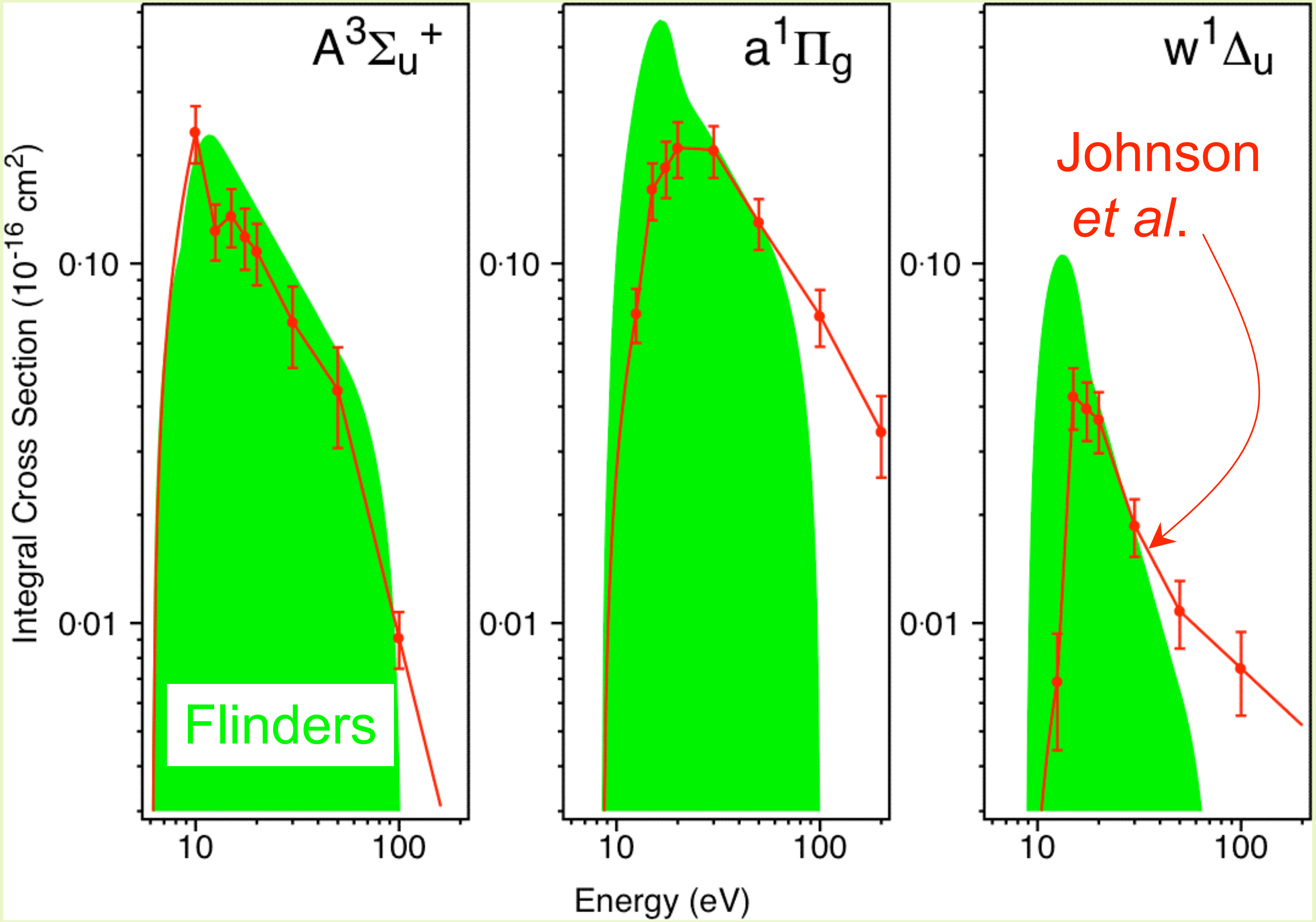
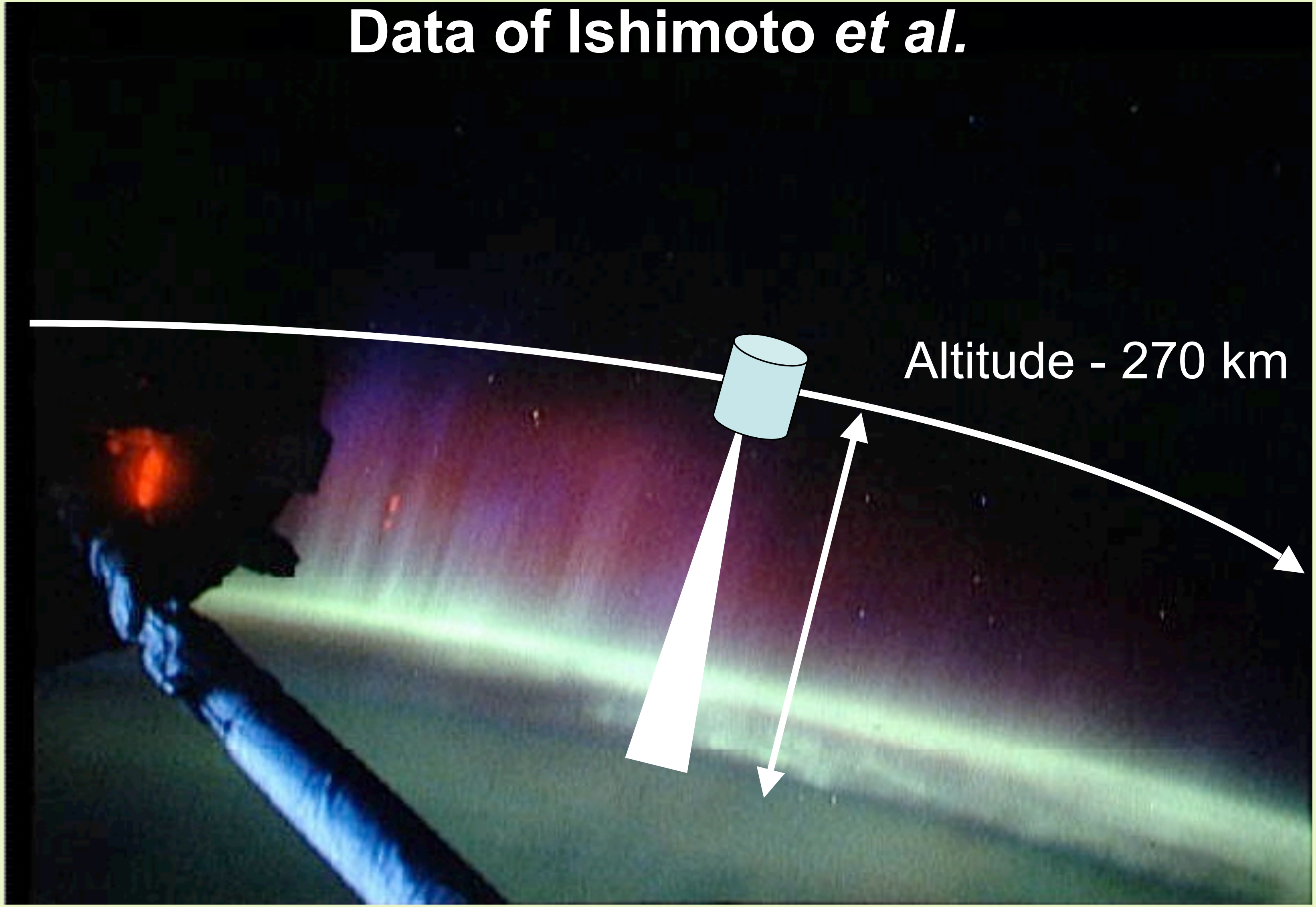
# Testing available cross section data bases: VUV Emission from $N_2$ (LBH and Vegard-Kaplan)

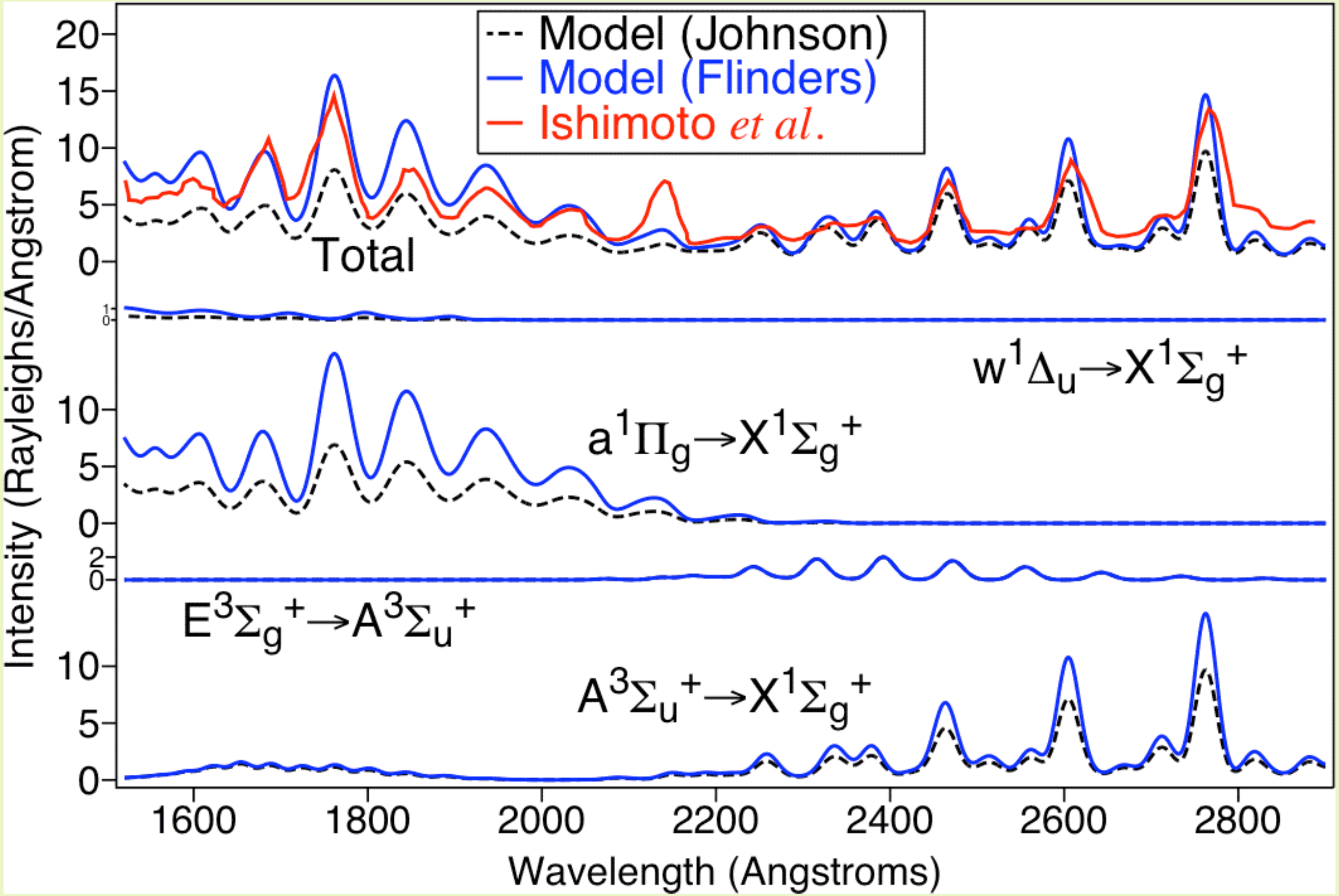


# VUV emission from $N_2$

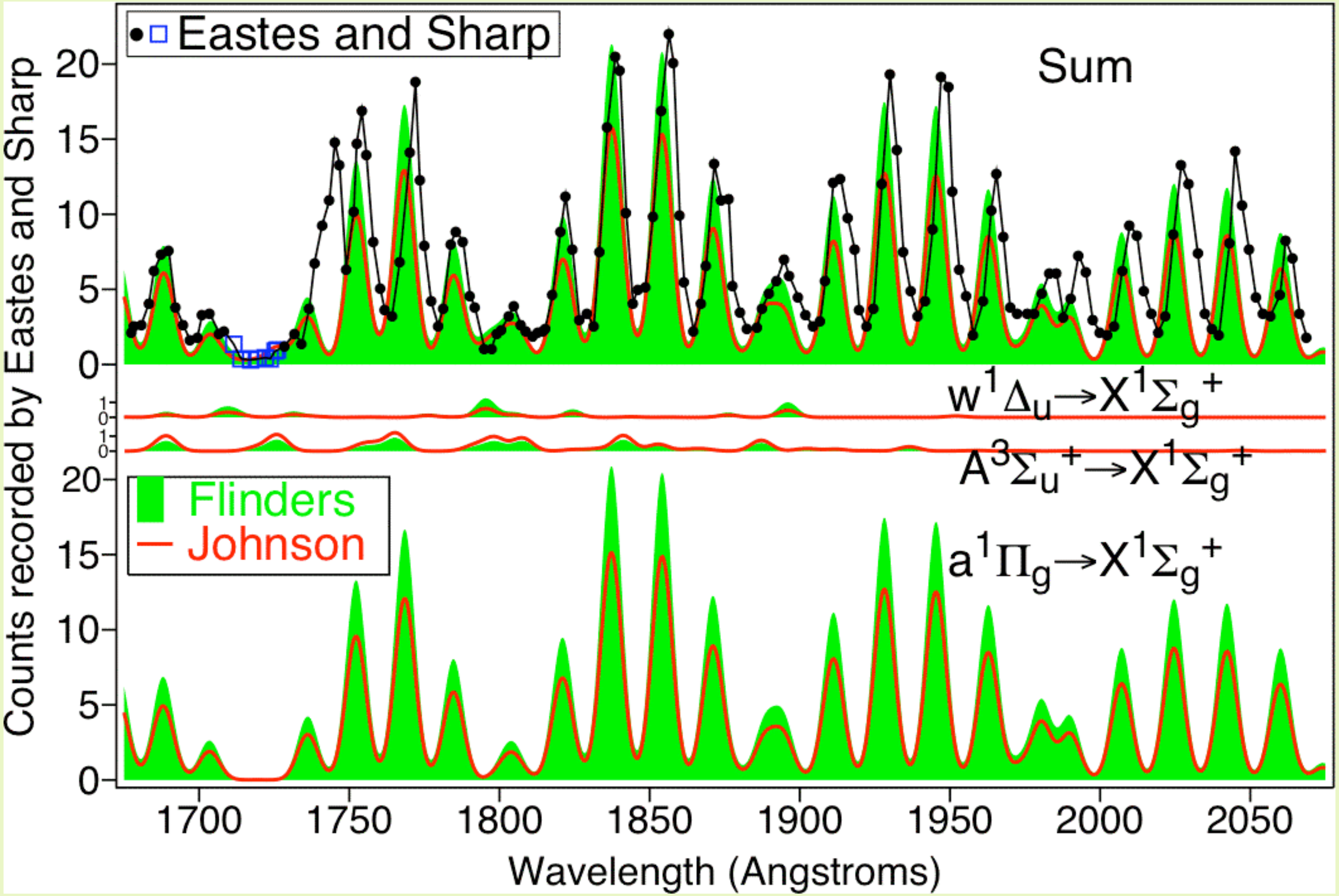
Data of Ishimoto *et al.*



# Comparison with measurements



# Comparison with high-res. measurements



# Electron density calculations

- Our model predicts an extended and non-Maxwell/Boltzmann distribution for $N_2^*(X^1\Sigma_g^+)$ populations.
- One way of testing this result is to compare our predictions against the International Reference Ionosphere (IRI) for the altitude dependence of the electron density.

# Vibrationally excited nitrogen

- It is believed that molecular nitrogen acts to reduce electron density by the reaction:

$$O^+ + N_2 \rightarrow NO^+ + N(^4S)$$

followed by the relatively rapid recombinations:

$$NO^+ + e^- \rightarrow N(^2D) + O$$

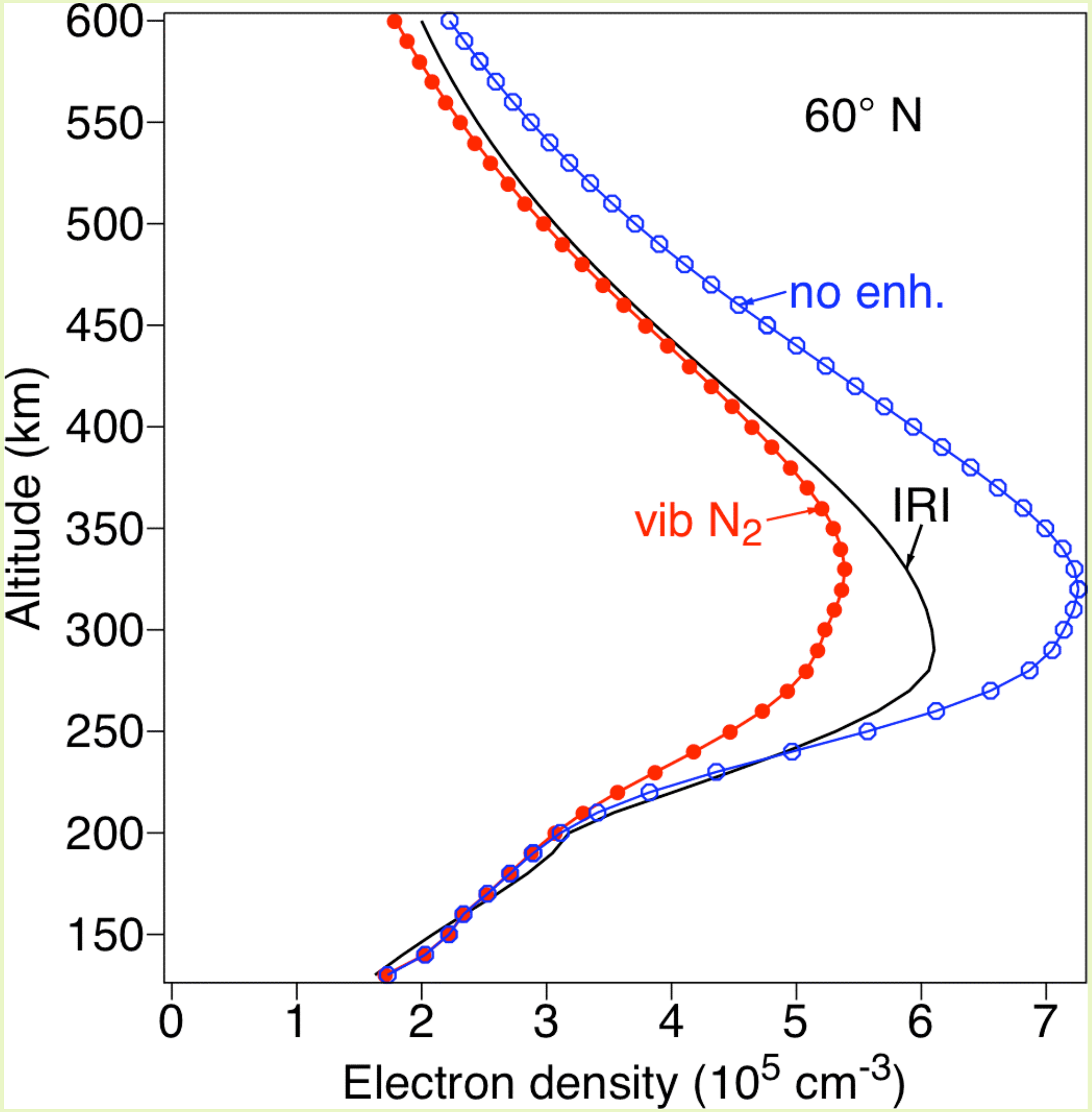
$$NO^+ + e^- \rightarrow N(^4S) + O$$

- With the first reaction proceeding much more rapidly if the molecular nitrogen is vibrationally excited:

$$O^+ + N_2[\nu'>1] \rightarrow NO^+ + N(^4S)$$

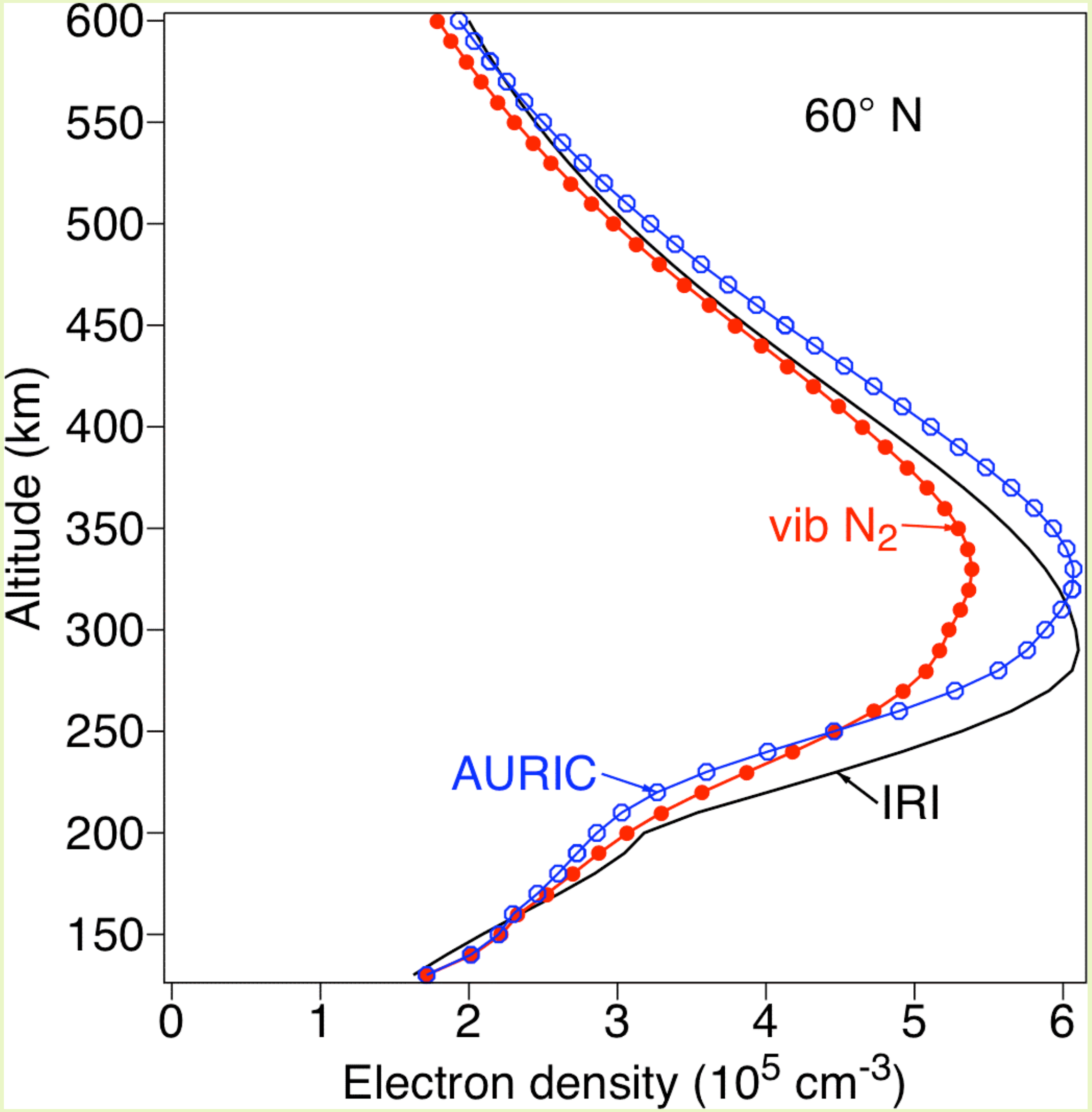
# Effect of Vibrationally Excited $N_2$

- Comparison of the calculated electron density versus altitude with the International Reference Ionosphere (IRI) for:
  - Enhancement due to vibrationally excited $N_2$ (●—●—●).
  - No enhancement (○—○—○).

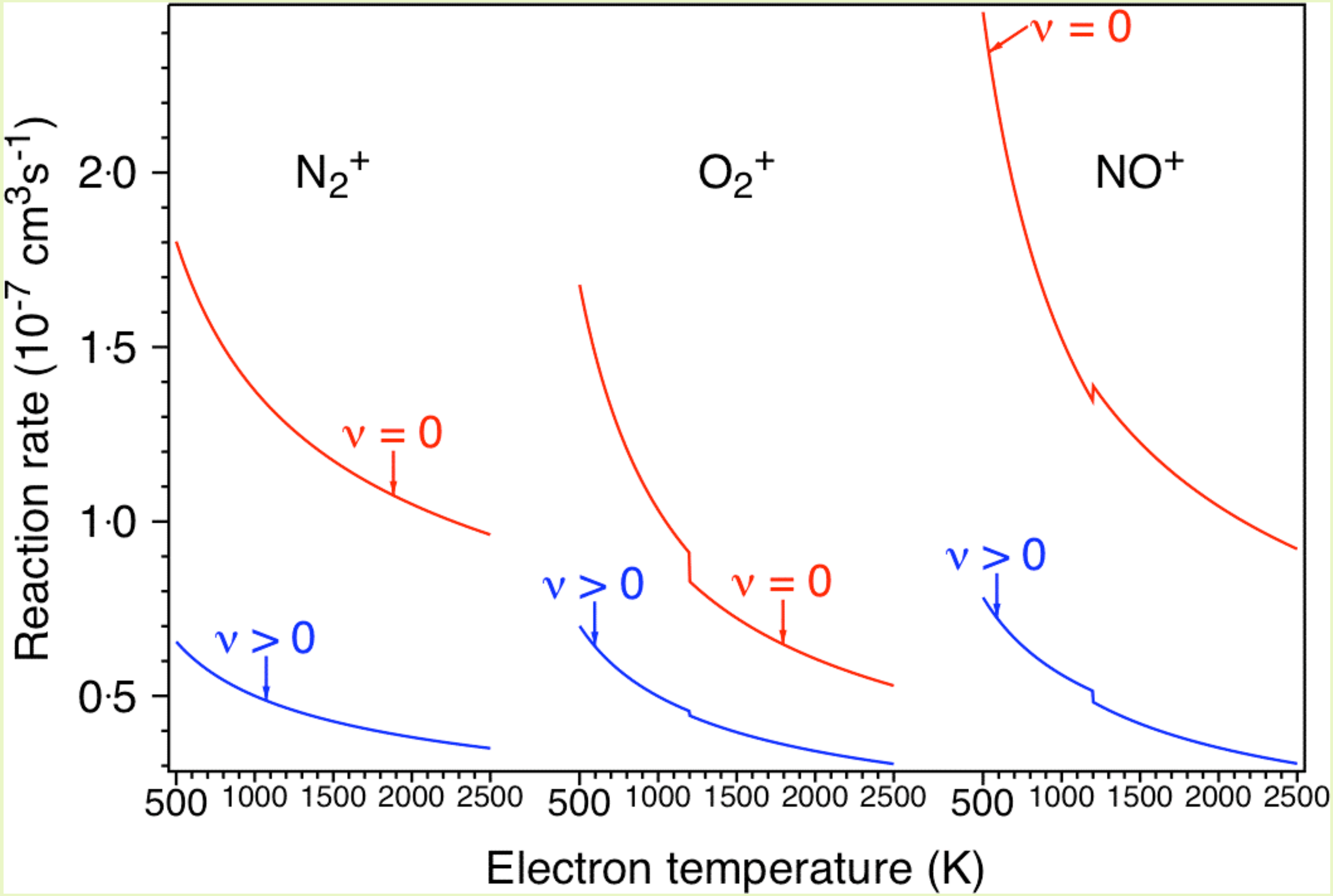


# Comparison with AURIC $N_2$* formula

- Comparison of Flinders (●—●—●) and AURIC (○—○—○) $N_2$* implementation:
  - “Flinders” case better at low and high altitudes.
  - Suggests rate constants for $N_2$* may be too high in range 250–350 km.



# Dissociative Recombination rates



# Importance of excited positive ions

- Comparison of calculated electron densities for:

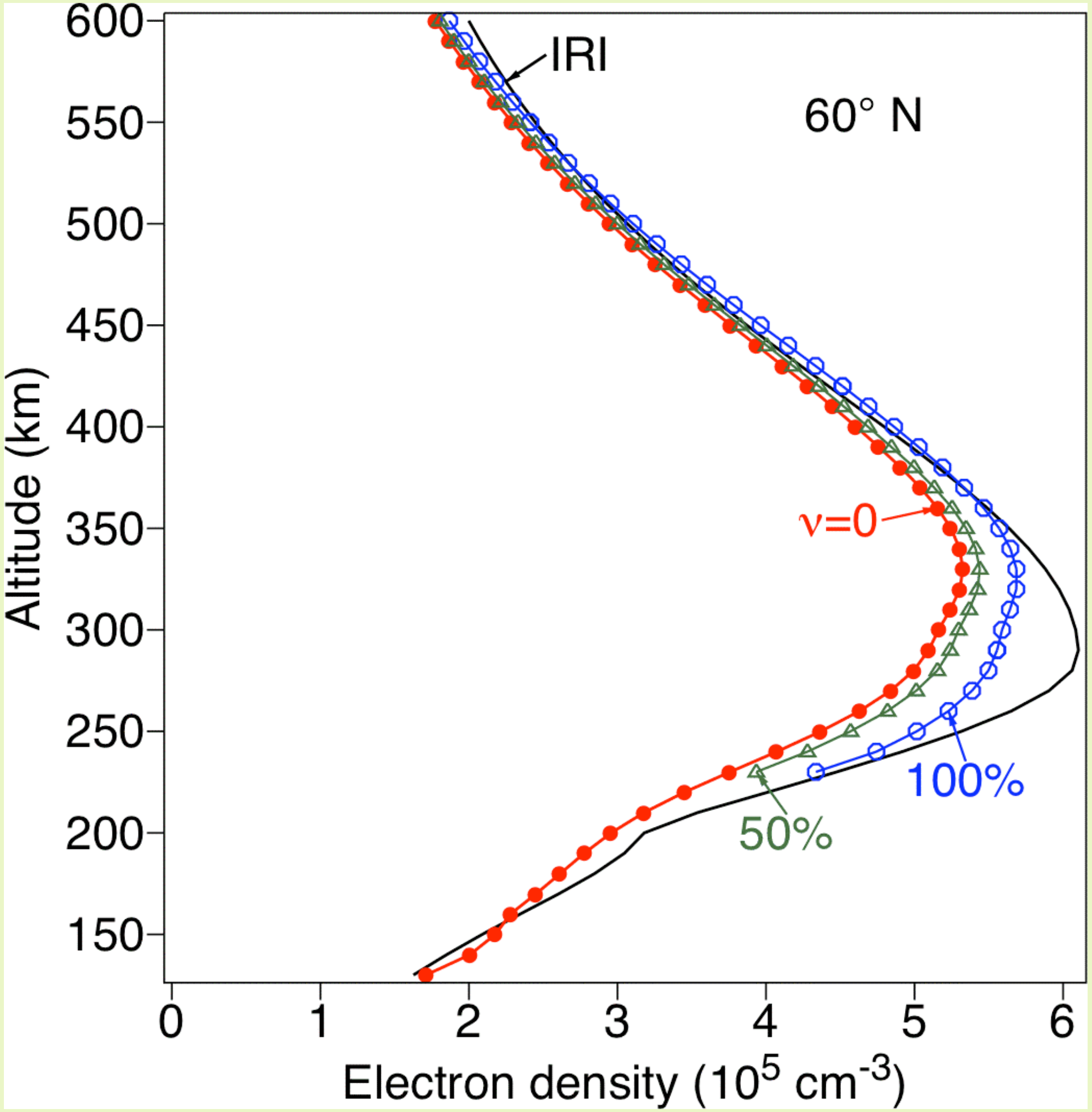
  zero (●—●—●),

  50% (△—△—△)

  and

  100%(○—○—○)

  excitation of $O_2^+$, $N_2^+$ and $NO^+$.



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# Conclusions

Accurate data bases for electron impact and photoionisation cross sections, transition probabilities, quenching rates, diffusion coefficients and chemical (neutral species and ions) reaction rates etc. are required to quantitatively model atmospheric phenomena. Some or our recent findings include:

- Infrared emission from NO
  - Electron impact shown to be as important as the chemiluminescent reaction at some altitudes.
- Prediction of VUV emissions
  - Better agreement with measurements using Flinders set of cross sections for $N_2$ excitation.

# Conclusions (cont.)

- Calculation of atmospheric electron density
  - Inclusion of effect of vibrationally excited $N_2$ improves agreement of calculated electron density with measurements.
  - Better results at some heights compared to Boltzmann distribution assumed in a standard atmospheric model.
  - Effect seems overestimated at height of peak electron density $\Rightarrow$ rate constants for $N_2^*$ too high here.
  - Vibrational level of positive ions in recombination may be significant.