

# Code comparison: Problem 1

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H. Frank and V. Bakshi



# Atomic kinetics of tin plasmas

## Problem 1

This problem explores the atomic kinetics of tin under conditions relevant for EUV production.

Participants were asked to compute the charge state distribution, absorptivity, emissivity, **spectral purity**, internal energy density and radiative power losses for cases shown below:

ID	1	2	3	4	5	6	7
$T_e$	10	15	20	25	30	35	40
$N_e$	$10^{19}$						

Critical electron density for CO<sub>2</sub> laser light

ID	8	9	10	11	12	13	14	15	16
$T_e$	20	25	30	35	40	45	50	55	60
$N_e$	$10^{20}$								

ID	17	18	19	20	21	22	23	24	25
$T_e$	20	25	30	35	40	45	50	55	60
$N_e$	$10^{21}$								

Critical electron density for Nd:YAG laser light

# Participants

We received **10** submissions for problem 1

Name	Institution	Code	non-LTE	LTE
Akira Sasaki	National Institute for Quantum and Radiological Sciences	JATOM		
Howard Scott	Lawrence Livermore National Laboratory	Cretin	x 3	
Ilya Vichev	Keldysh Institute for Applied Mathematics	THERMOS		
Igor Golovkin	Prism Computational Sciences	PrismSPECT		
John Sheil	Advanced Research Center for Nanolithography	ATOMIC		
Hilik Frank	Lawrence Livermore National Laboratory	SEMILLAC		

- Compare key quantities (average charge state, spectral purity, etc.) for each electron density group.
- Global comparison of internal energy density and radiative power losses.

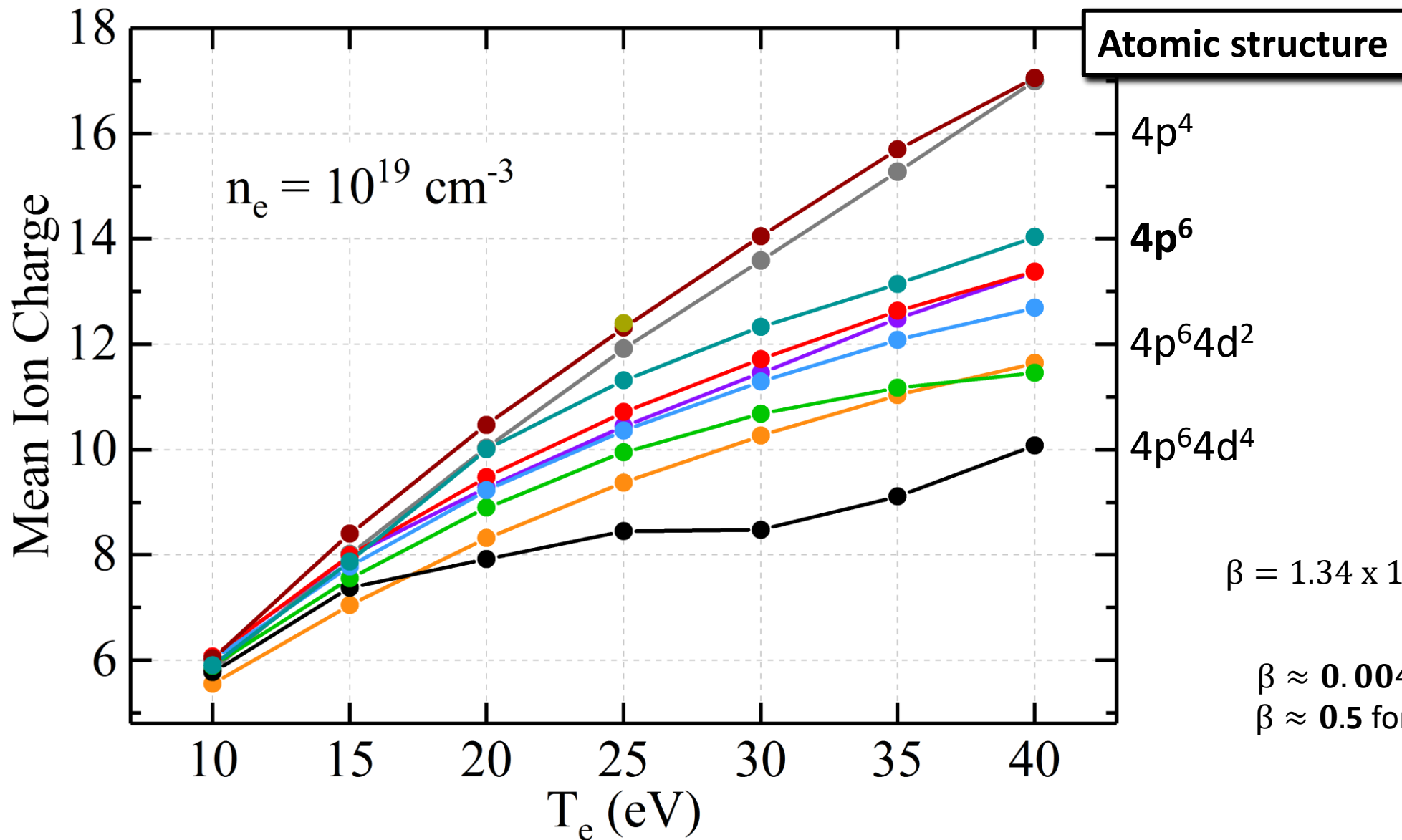
ID	1	2	3	4	5	6	7
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$N_e$	$10^{19}$						

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ID	17	18	19	20	21	22	23	24	25
$T_e$	20	25	30	35	40	45	50	55	60
$N_e$	$10^{21}$								

$$n_e = 10^{19} \text{ cm}^{-3}$$

# $n_e = 10^{19} \text{ cm}^{-3}$ : Mean charge state



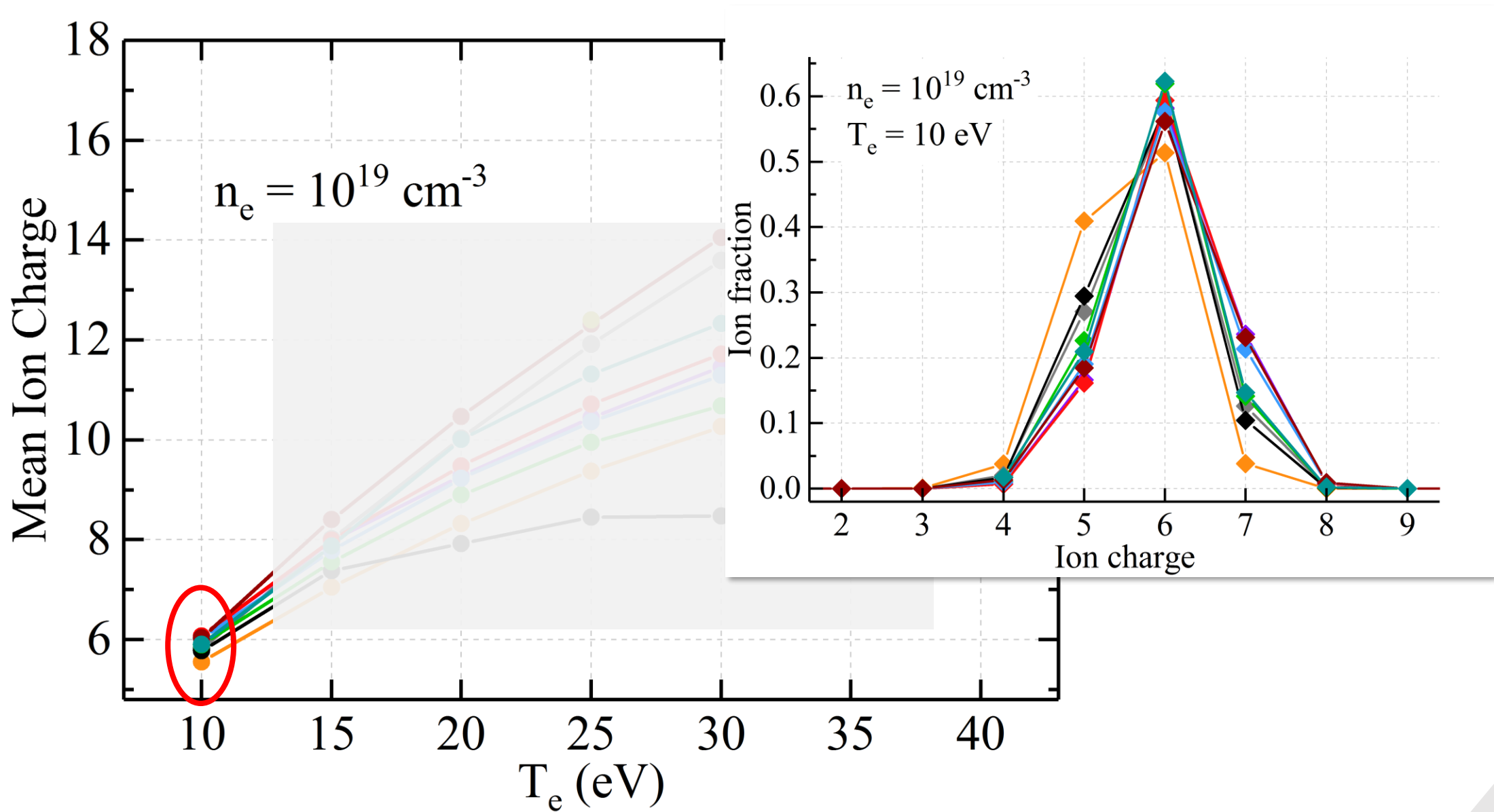
Atomic structure

- $4p^4$
- $4p^6$
- $4p^6 4d^2$
- $4p^6 4d^4$

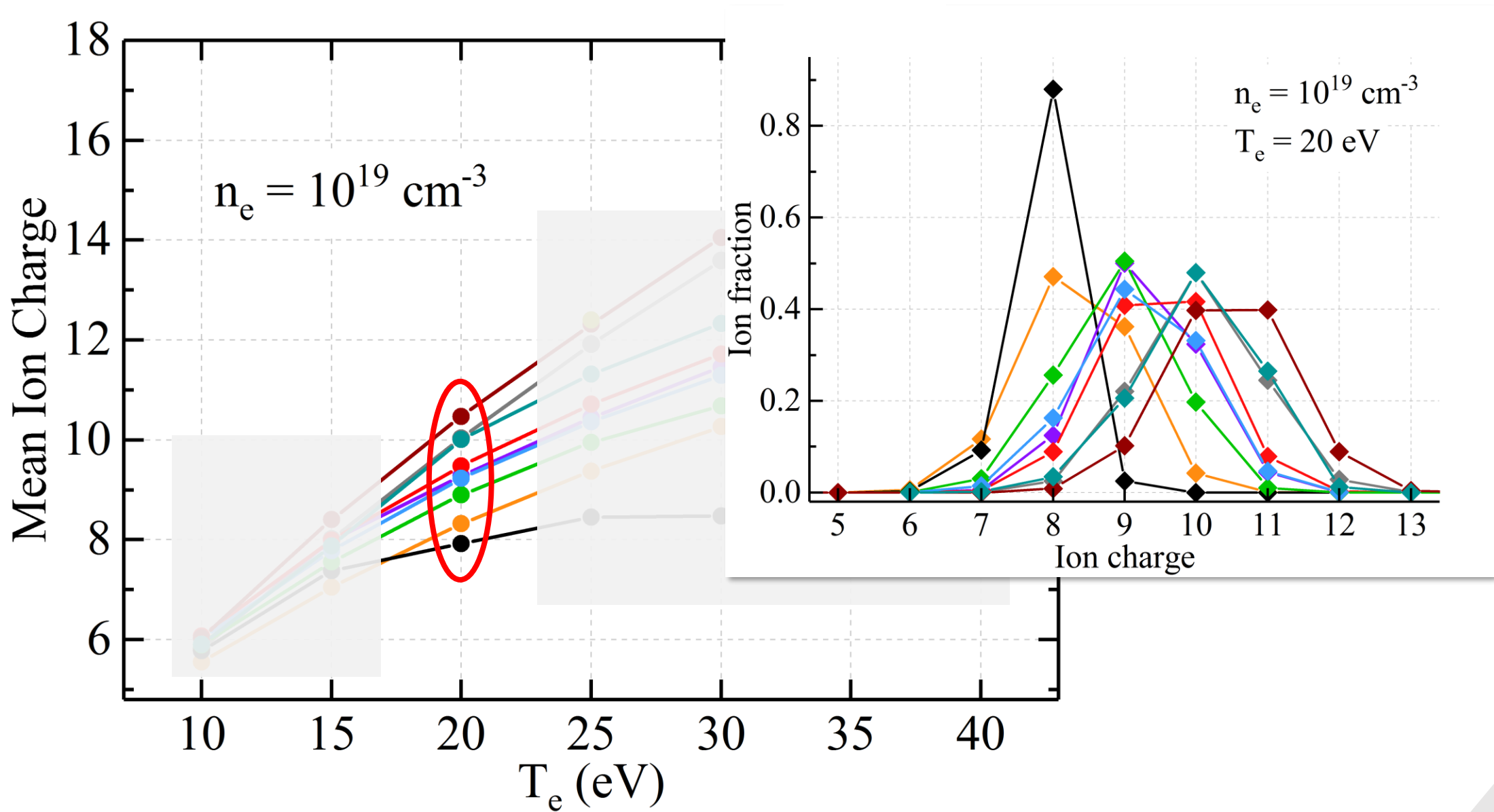
$$\beta = 1.34 \times 10^{13} \frac{T_e^{7/2}}{n_e} \ll 1 \text{ for LTE conditions}$$

$\beta \approx 0.004$  for  $T_e = 10 \text{ eV}$   
 $\beta \approx 0.5$  for  $T_e = 40 \text{ eV}$

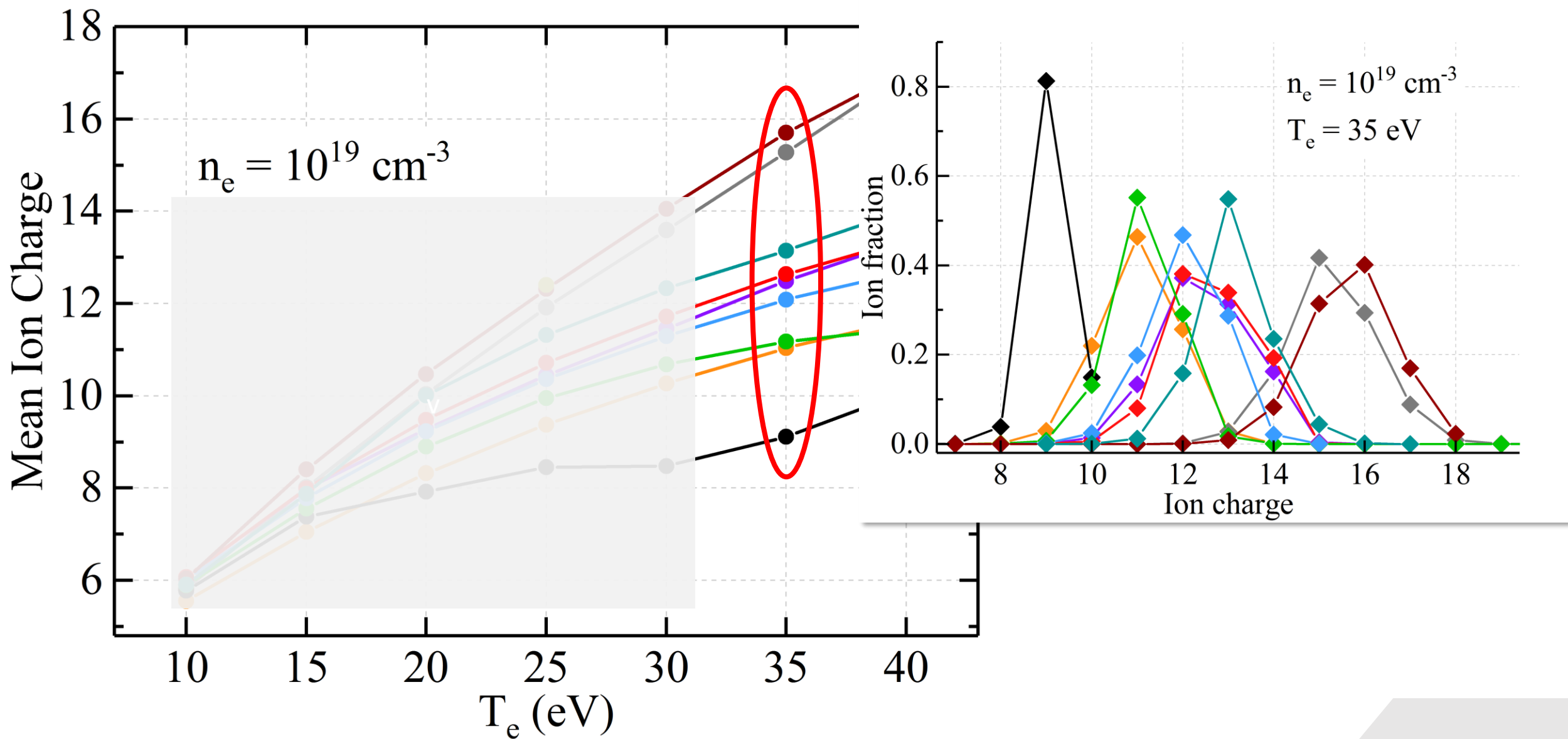
# $n_e = 10^{19} \text{ cm}^{-3}$ : Ion fraction



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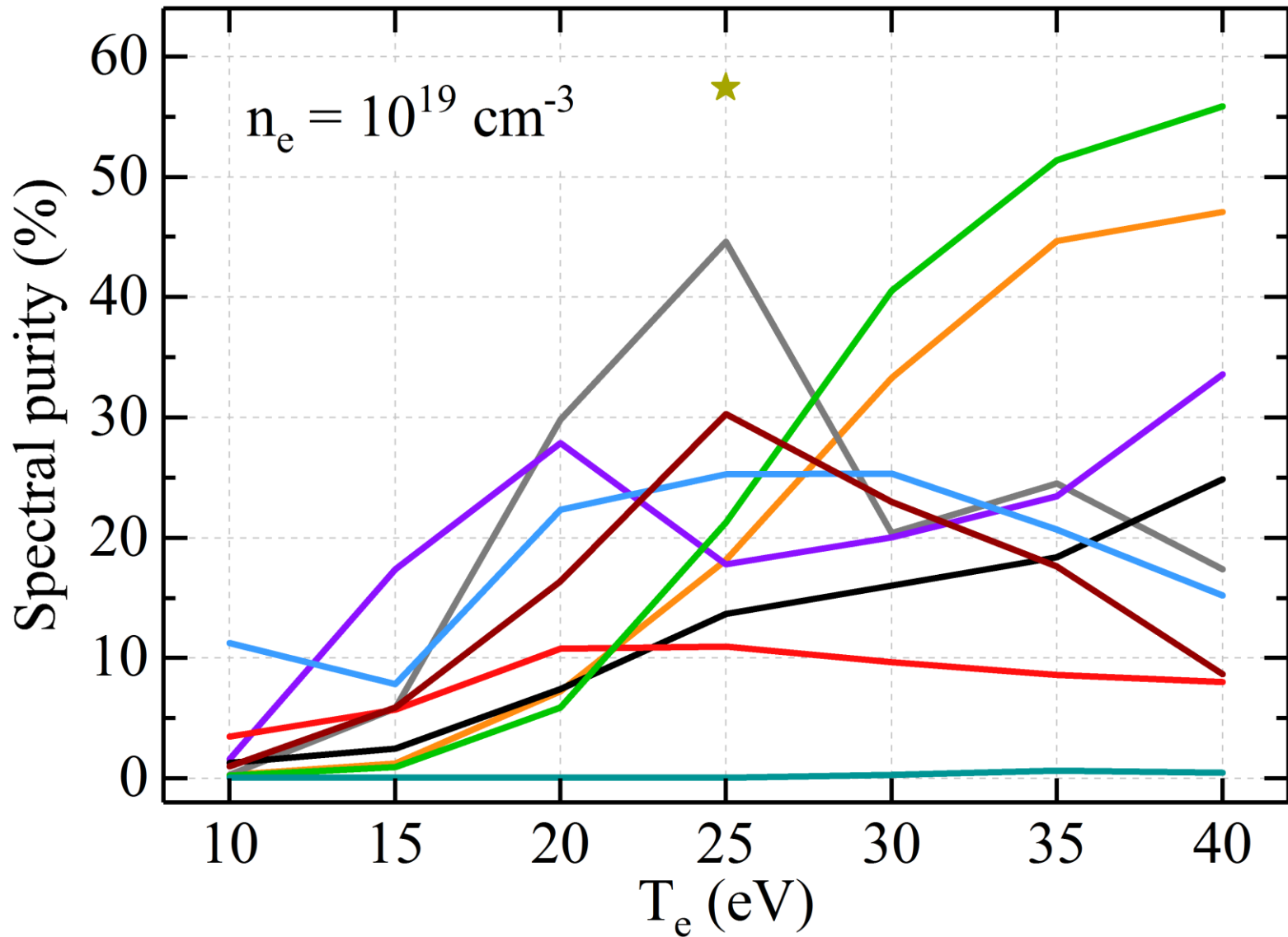


# $n_e = 10^{19} \text{ cm}^{-3}$ : Ion fraction



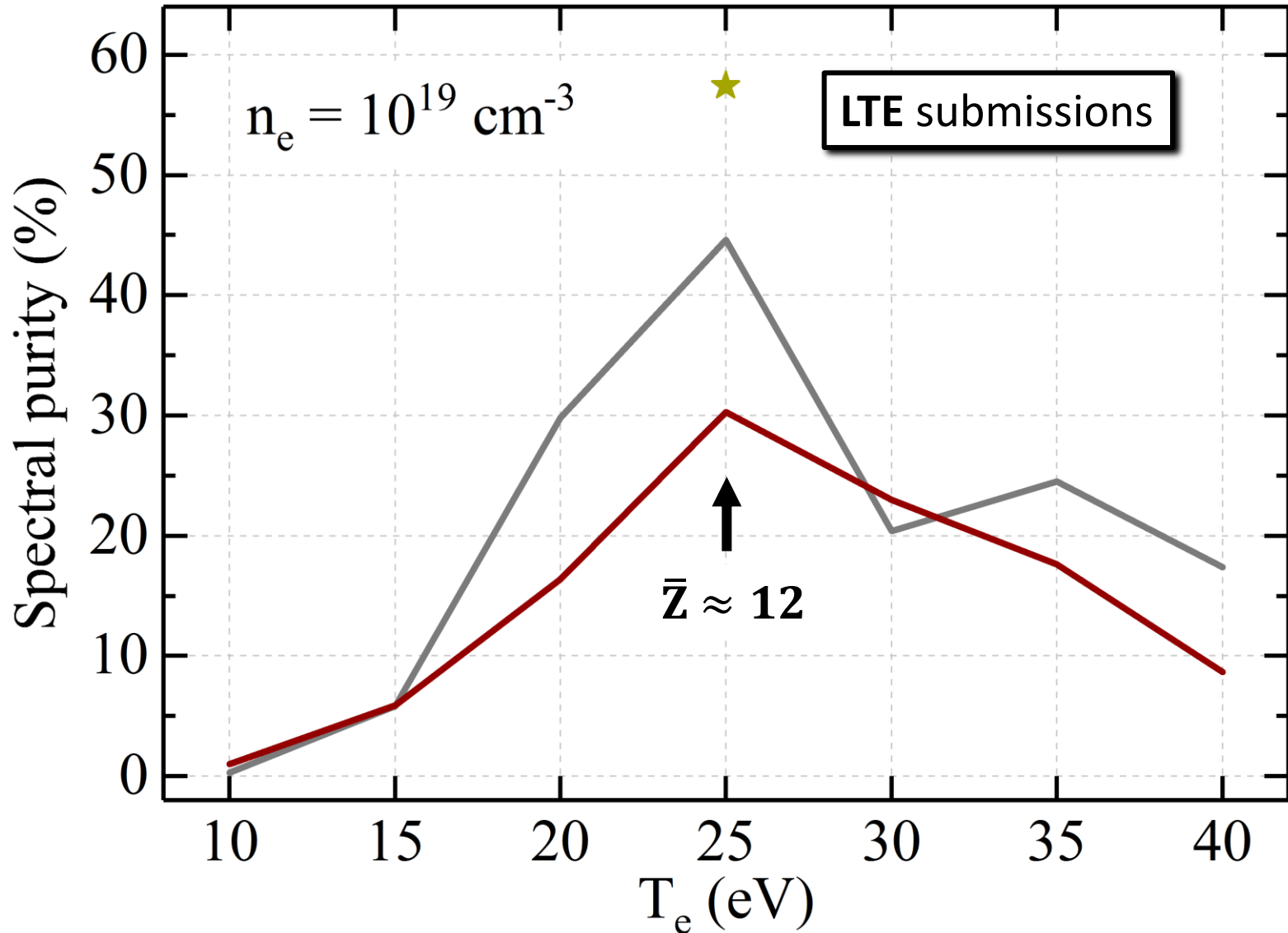


# $n_e = 10^{19} \text{ cm}^{-3}$ : Spectral purity



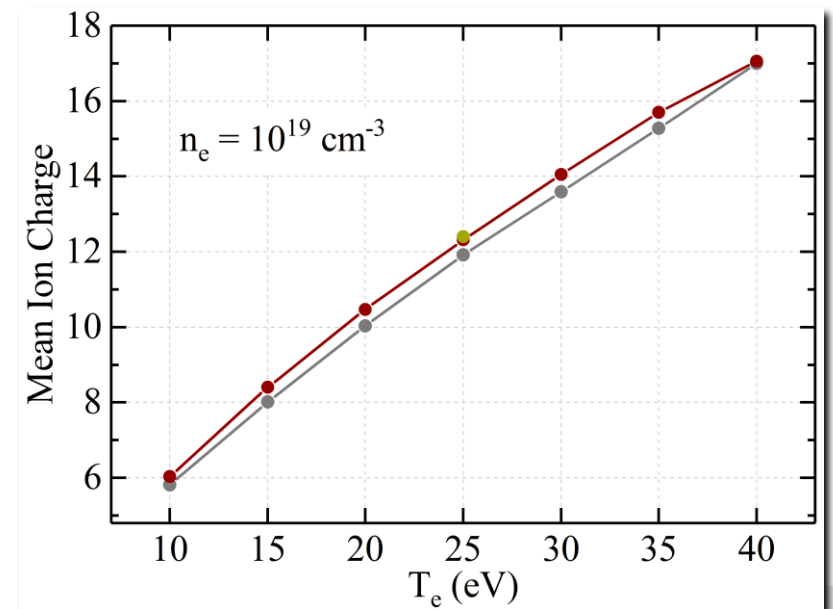
$$\text{Spectral purity} = \frac{\int_{13.365}^{13.635} \eta_{\lambda} d\lambda}{\int_5^{20} \eta_{\lambda} d\lambda}$$

# $n_e = 10^{19} \text{ cm}^{-3}$ : Spectral purity

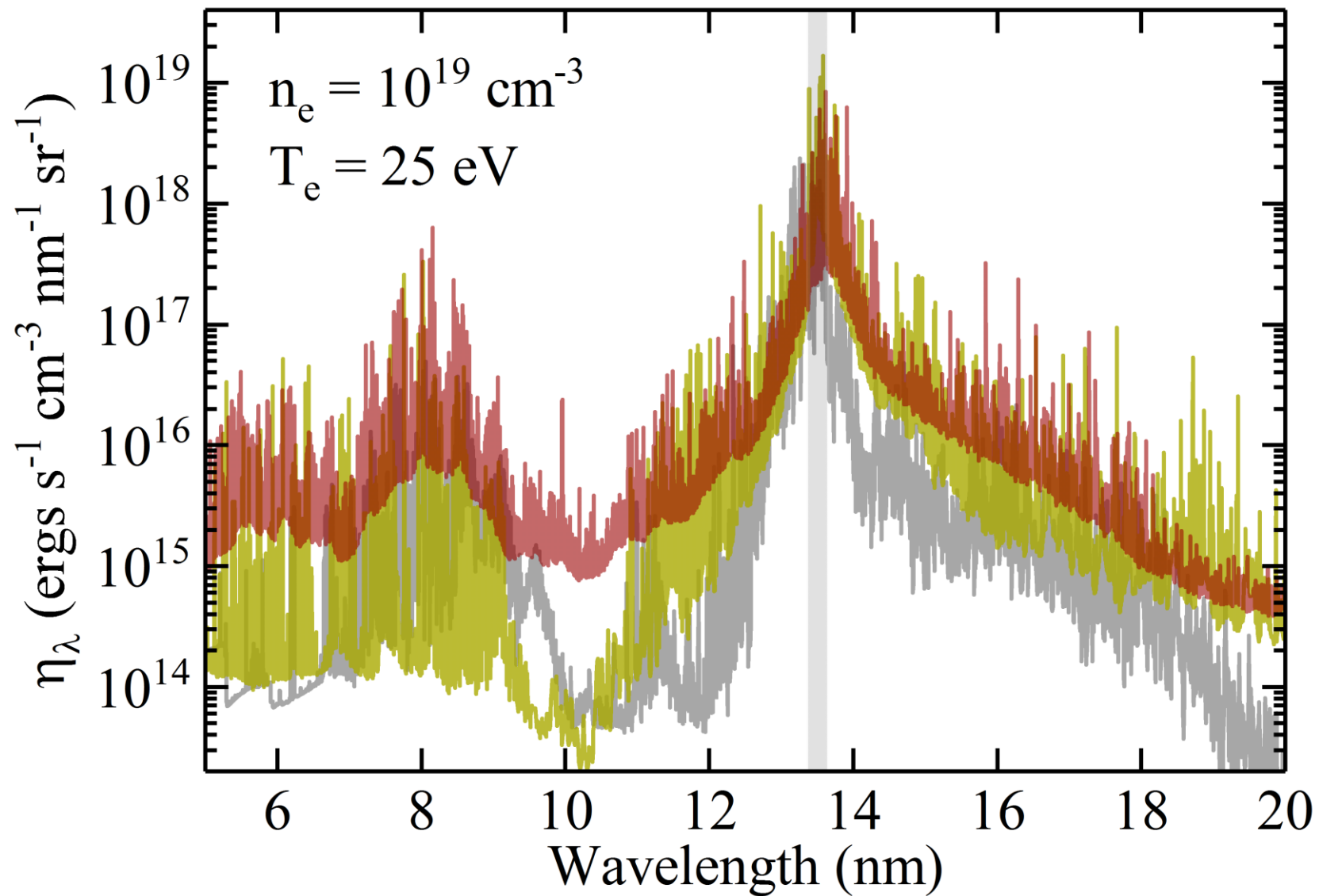


$$\text{Spectral purity} = \frac{\int_{13.365}^{13.635} \eta_{\lambda} d\lambda}{\int_5^{20} \eta_{\lambda} d\lambda}$$

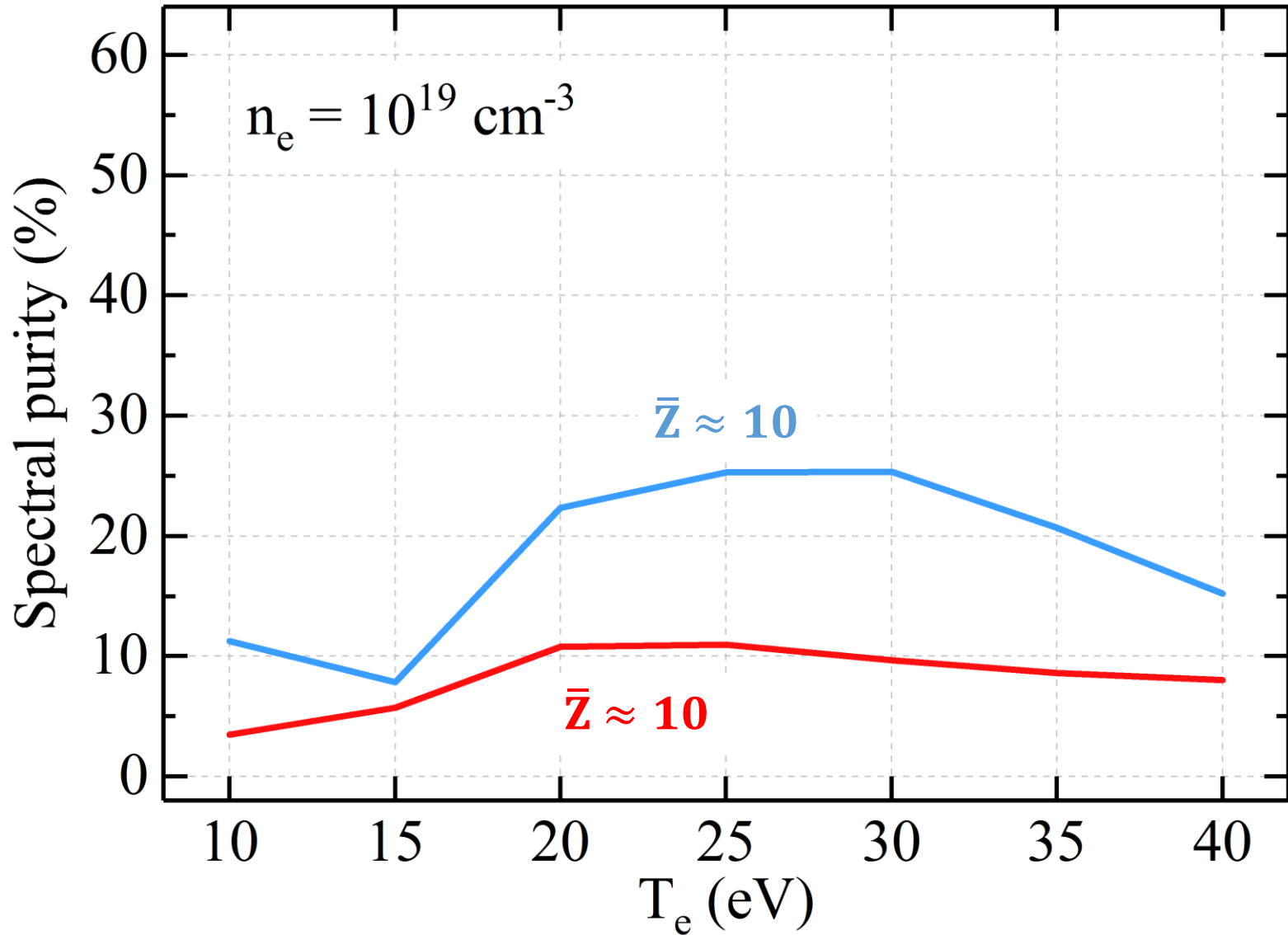
Peak in SP when  $\bar{Z} \approx 12$



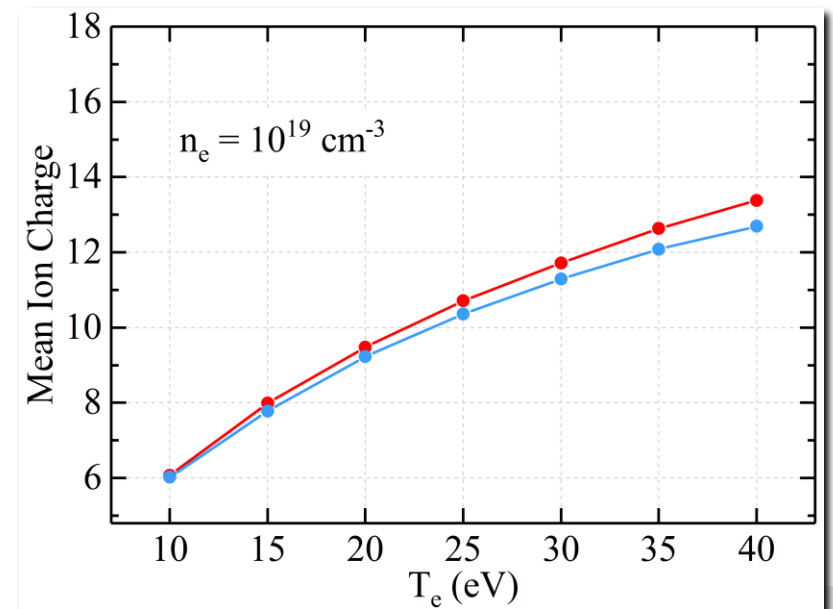
# $n_e = 10^{19} \text{ cm}^{-3}$ : Emissivity



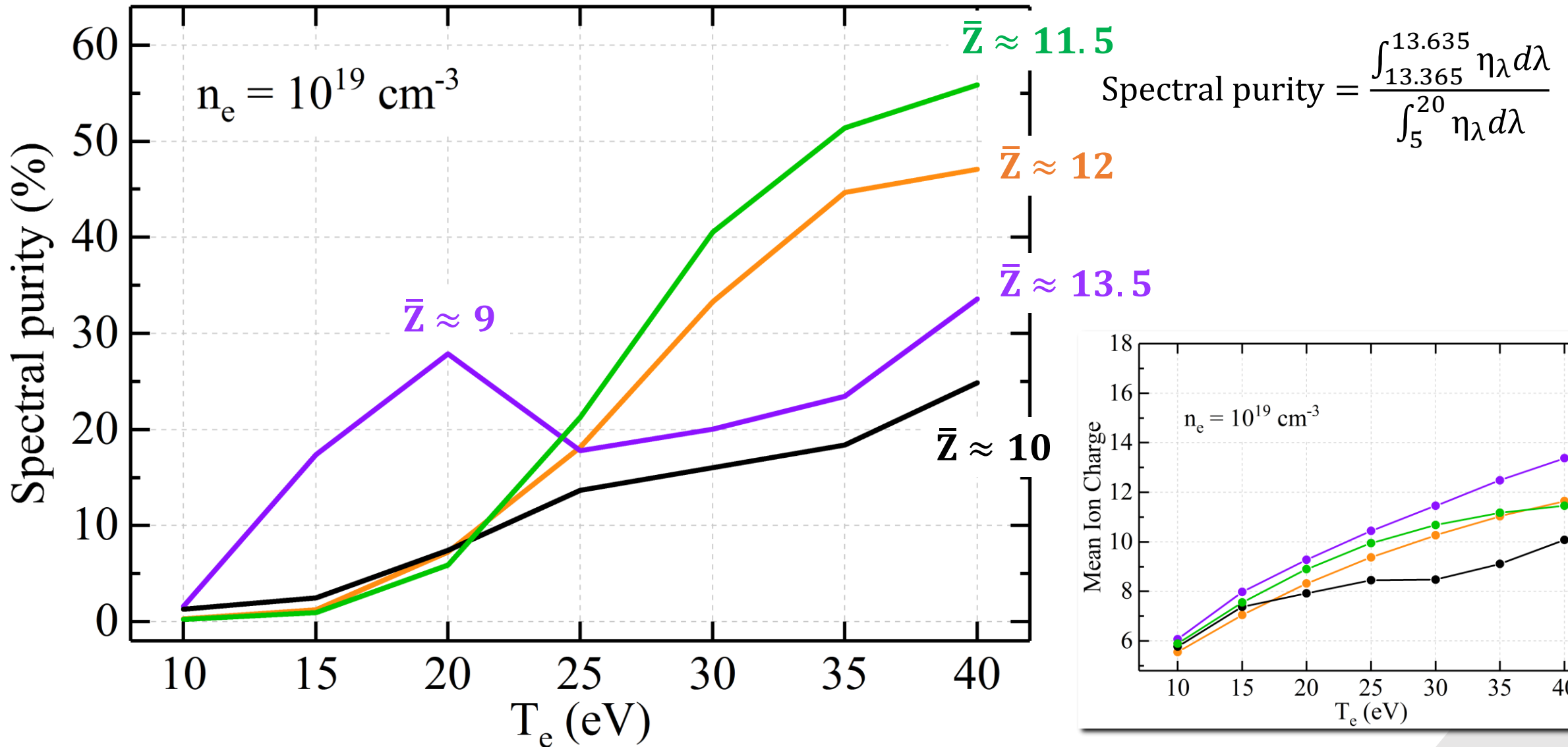
# $n_e = 10^{19} \text{ cm}^{-3}$ : Spectral purity



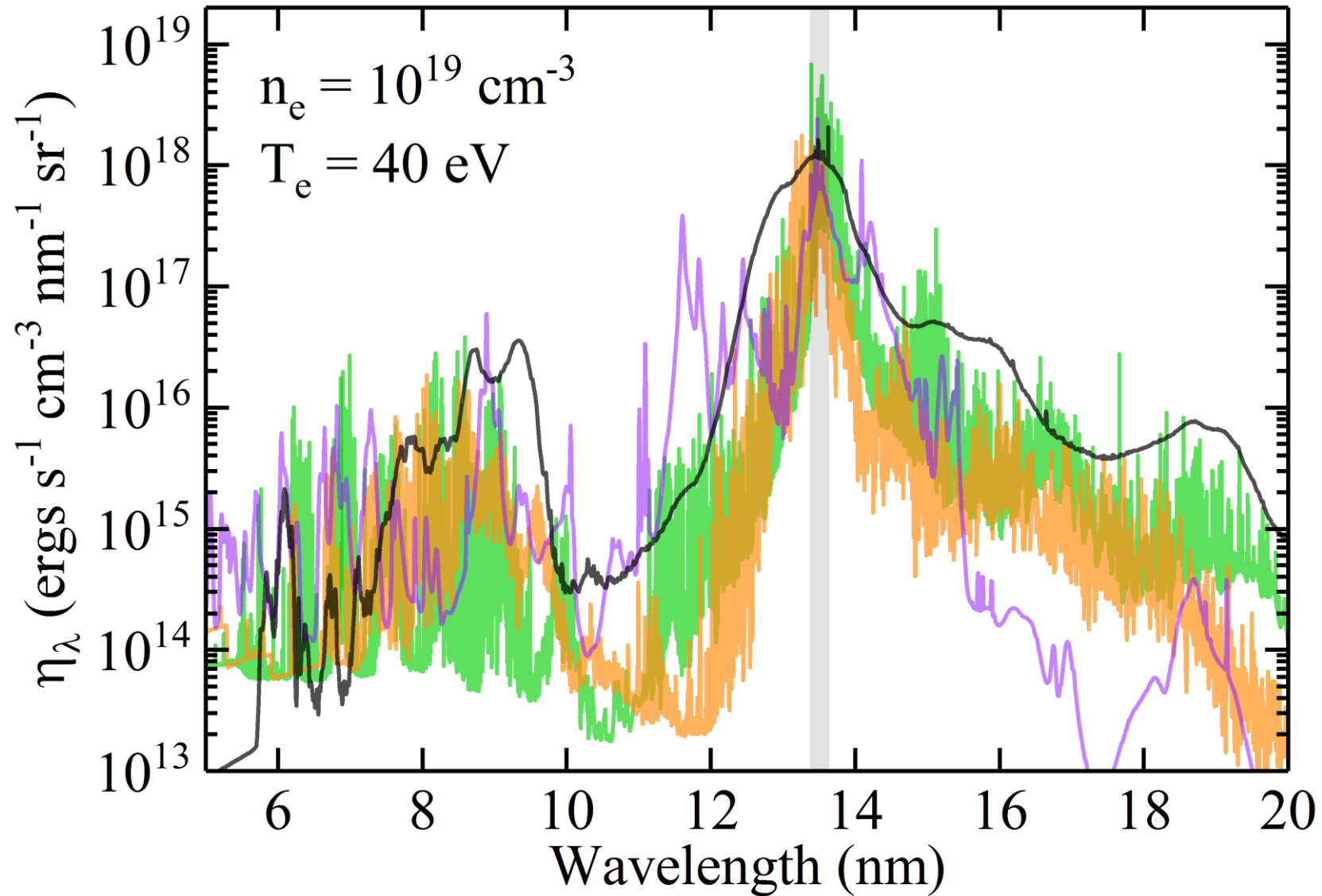
$$\text{Spectral purity} = \frac{\int_{13.365}^{13.635} \eta_{\lambda} d\lambda}{\int_5^{20} \eta_{\lambda} d\lambda}$$



# $n_e = 10^{19} \text{ cm}^{-3}$ : Spectral purity

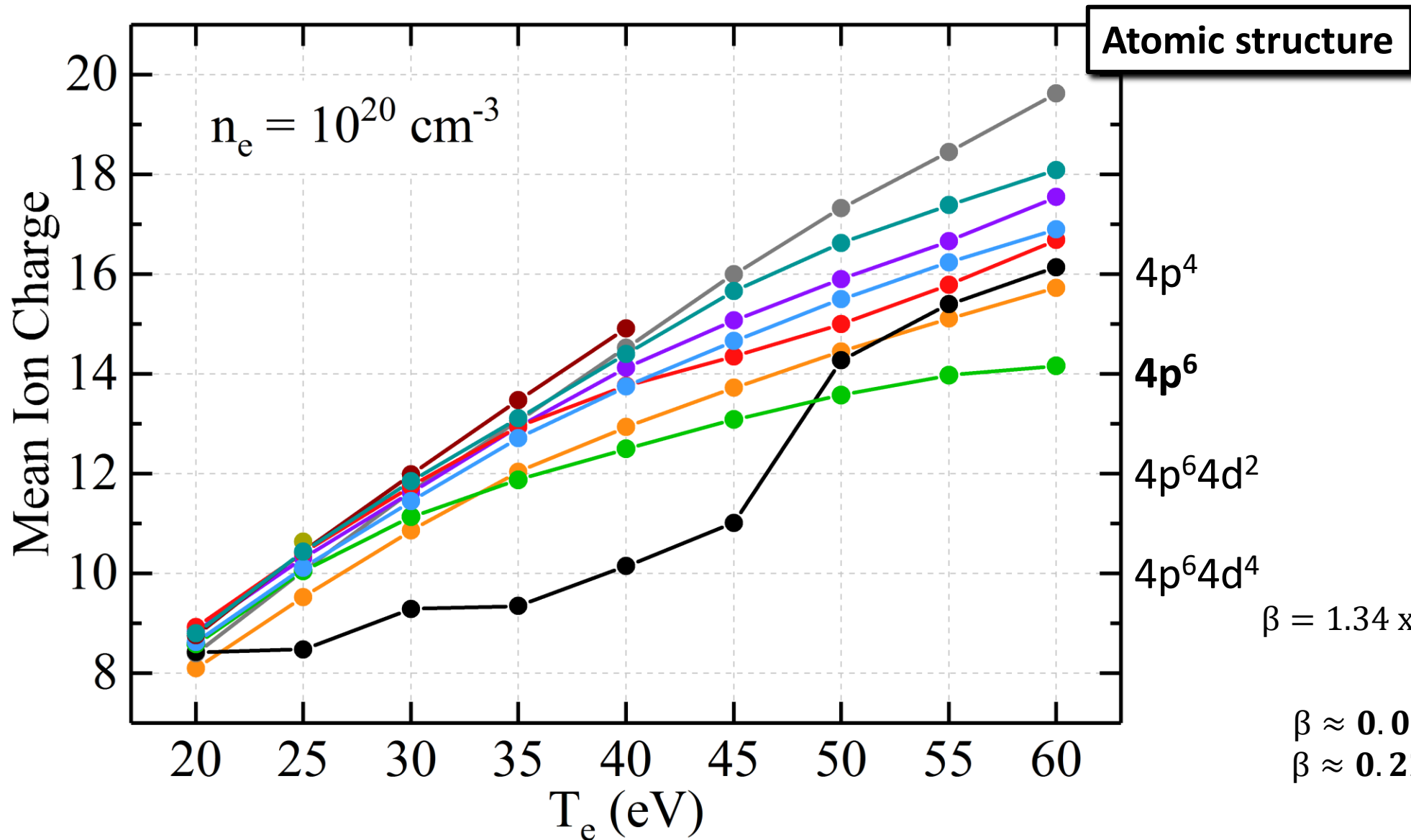


# $n_e = 10^{19} \text{ cm}^{-3}$ : Emissivity



$$n_e = 10^{20} \text{ cm}^{-3}$$

# $n_e = 10^{20} \text{ cm}^{-3}$ : Mean charge state



Atomic structure

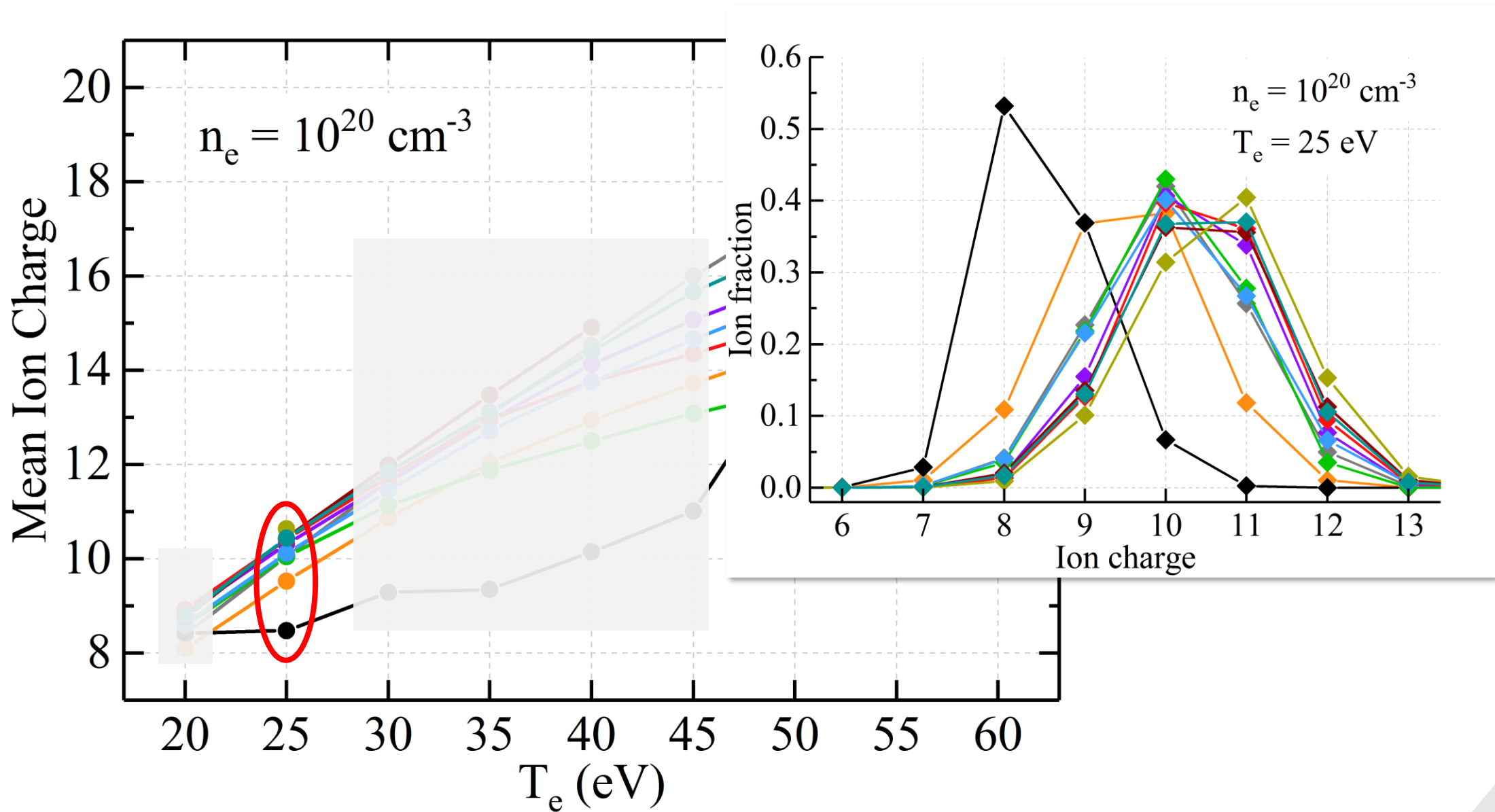
$$\beta = 1.34 \times 10^{13} \frac{T_e^{7/2}}{n_e} \ll 1 \text{ for LTE conditions}$$

$\beta \approx 0.005$  for  $T_e = 20 \text{ eV}$

$\beta \approx 0.22$  for  $T_e = 60 \text{ eV}$

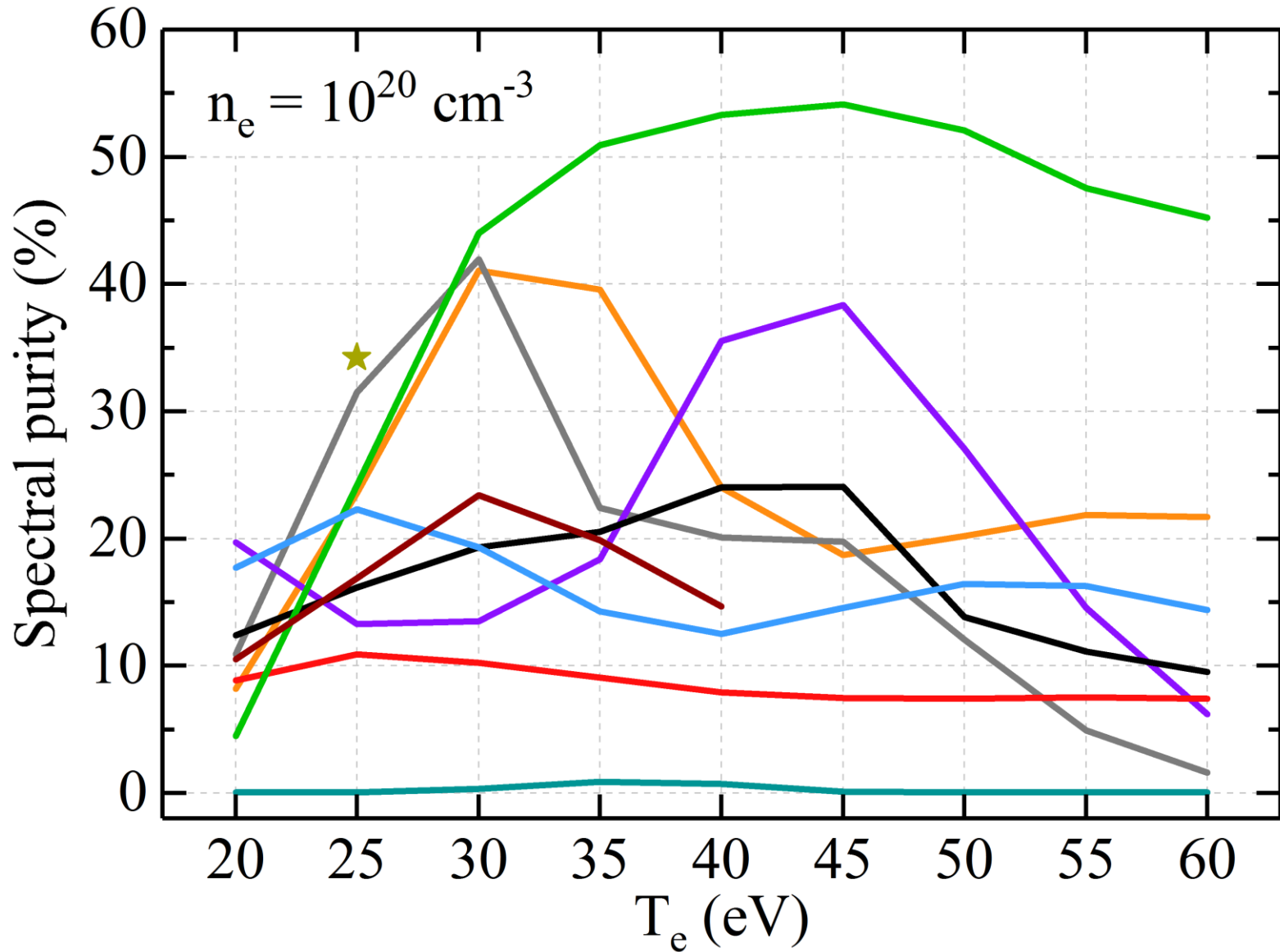


# $n_e = 10^{20} \text{ cm}^{-3}$ : Ion fraction



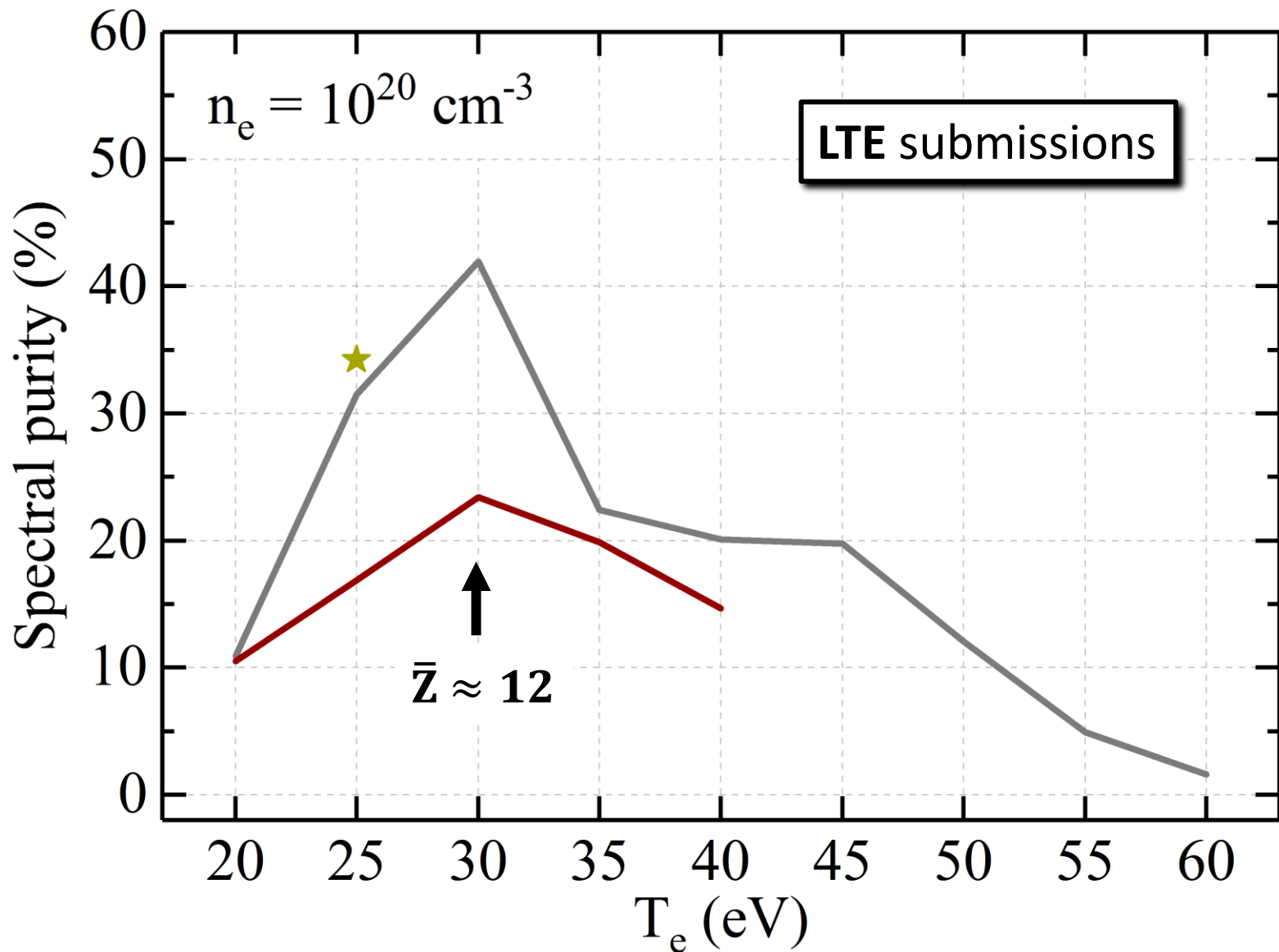


# $n_e = 10^{20} \text{ cm}^{-3}$ : Spectral purity

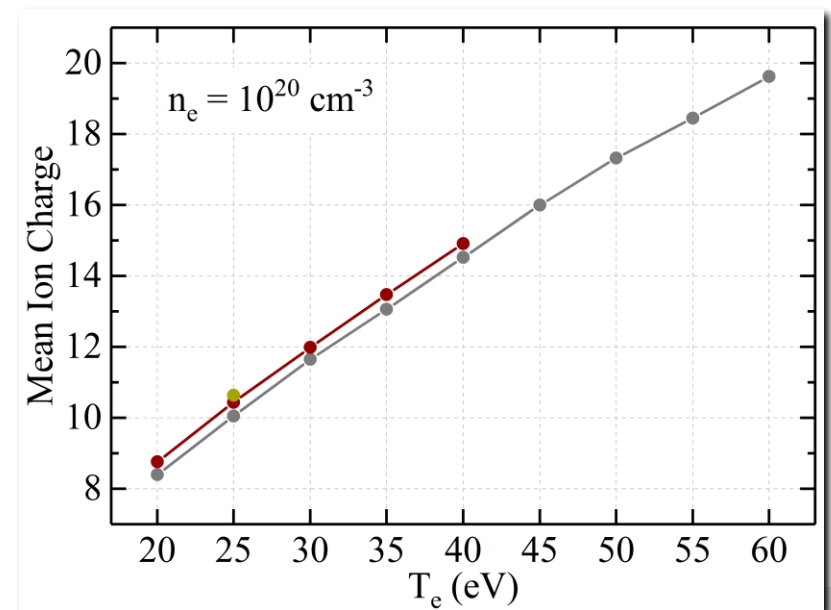


$$\text{Spectral purity} = \frac{\int_{13.365}^{13.635} \eta_{\lambda} d\lambda}{\int_5^{20} \eta_{\lambda} d\lambda}$$

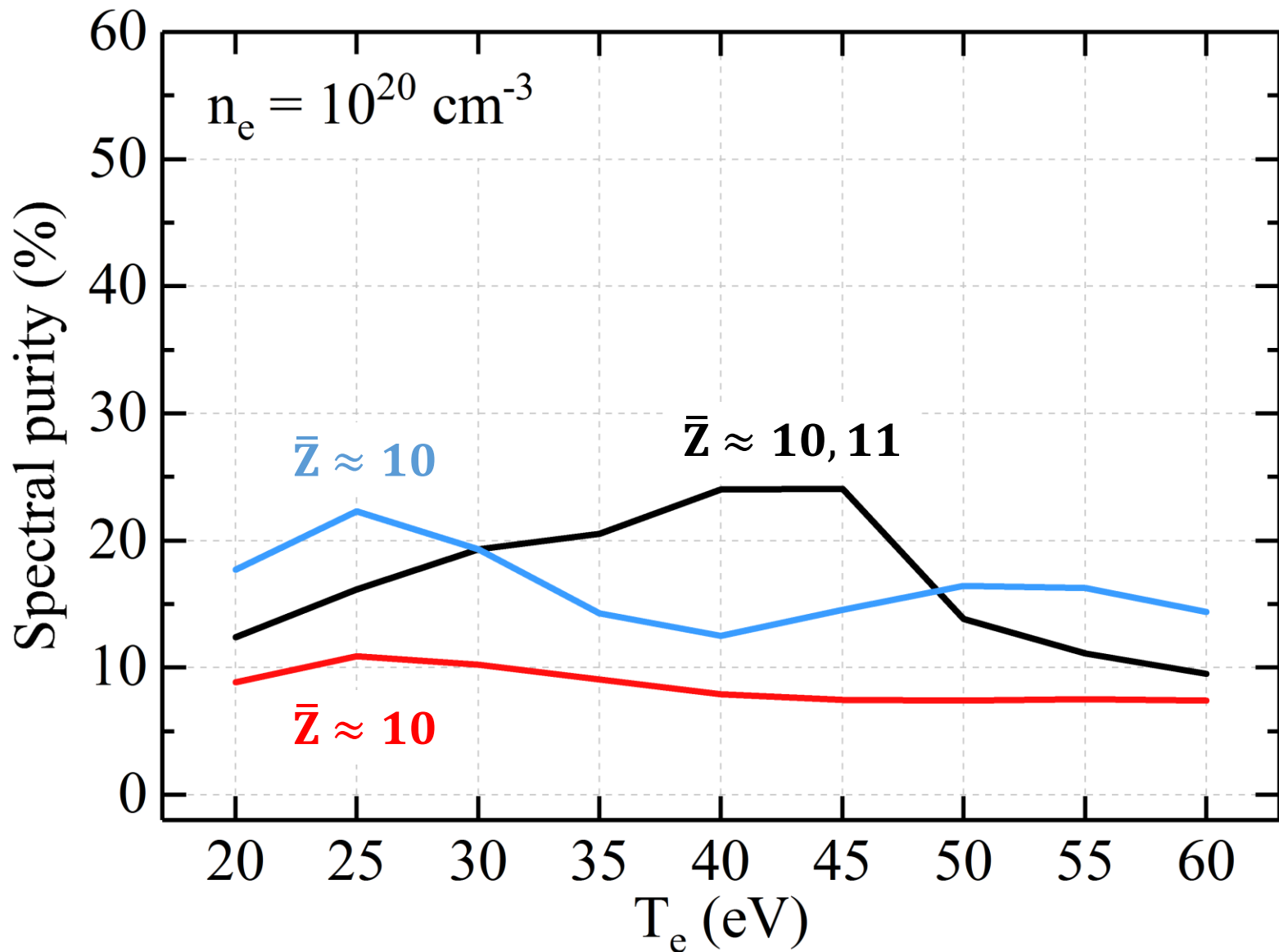
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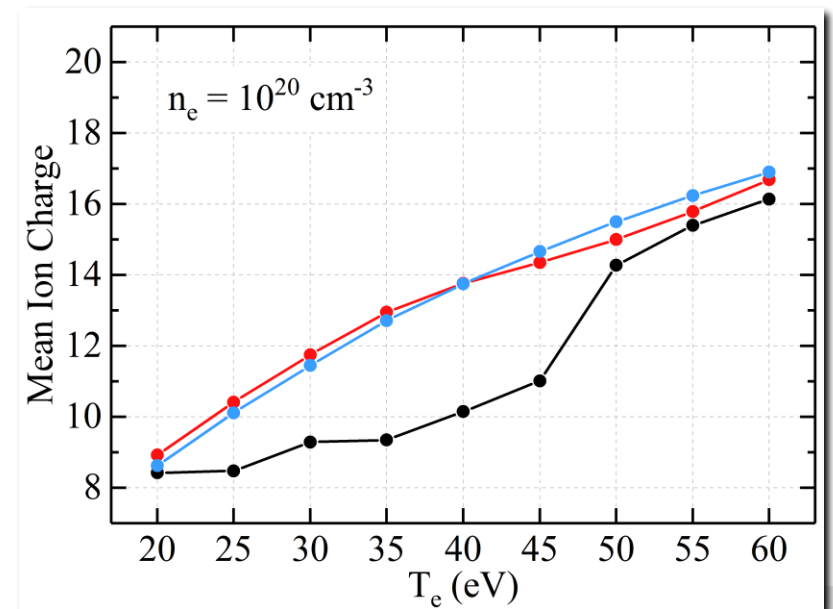
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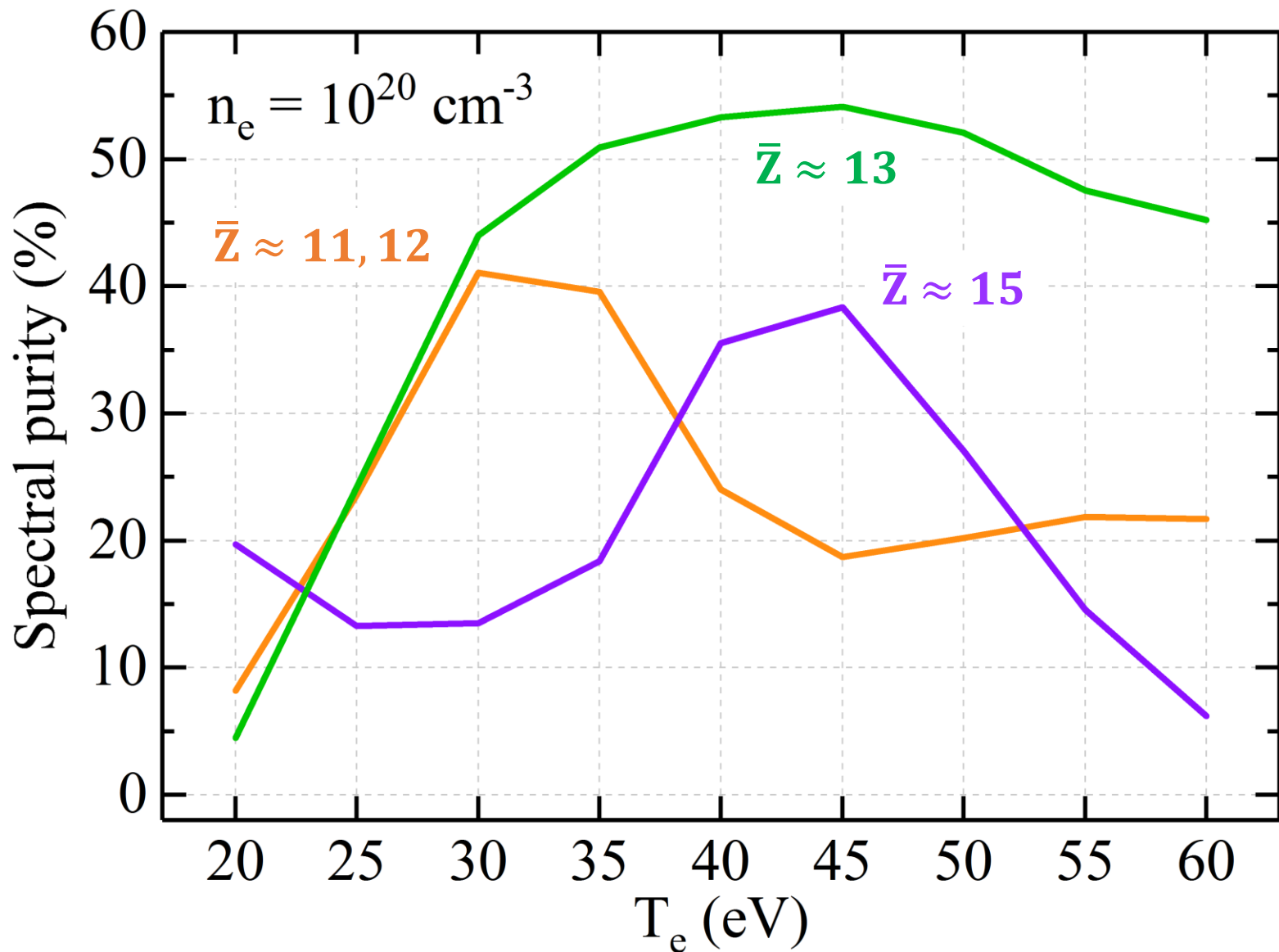
# $n_e = 10^{20} \text{ cm}^{-3}$ : Spectral purity



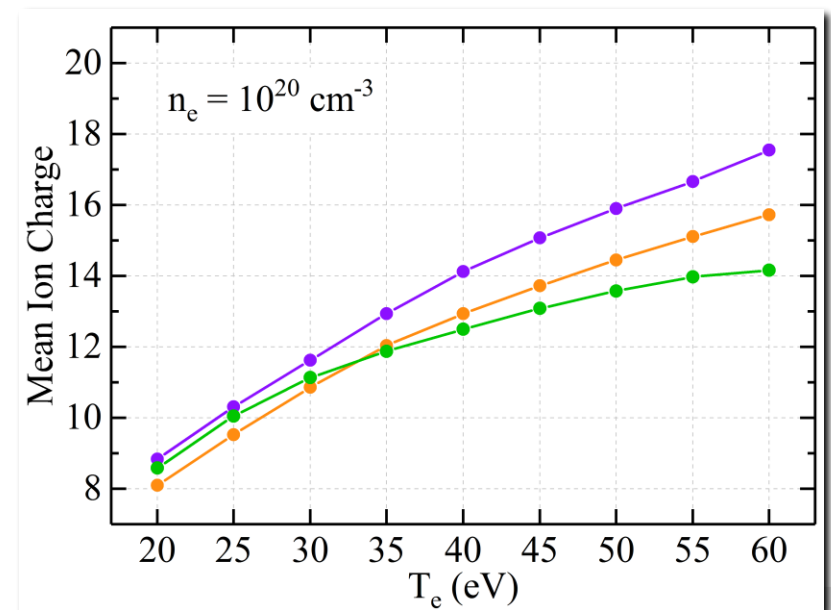
$$\text{Spectral purity} = \frac{\int_{13.365}^{13.635} \eta_\lambda d\lambda}{\int_5^{20} \eta_\lambda d\lambda}$$



# $n_e = 10^{20} \text{ cm}^{-3}$ : Spectral purity

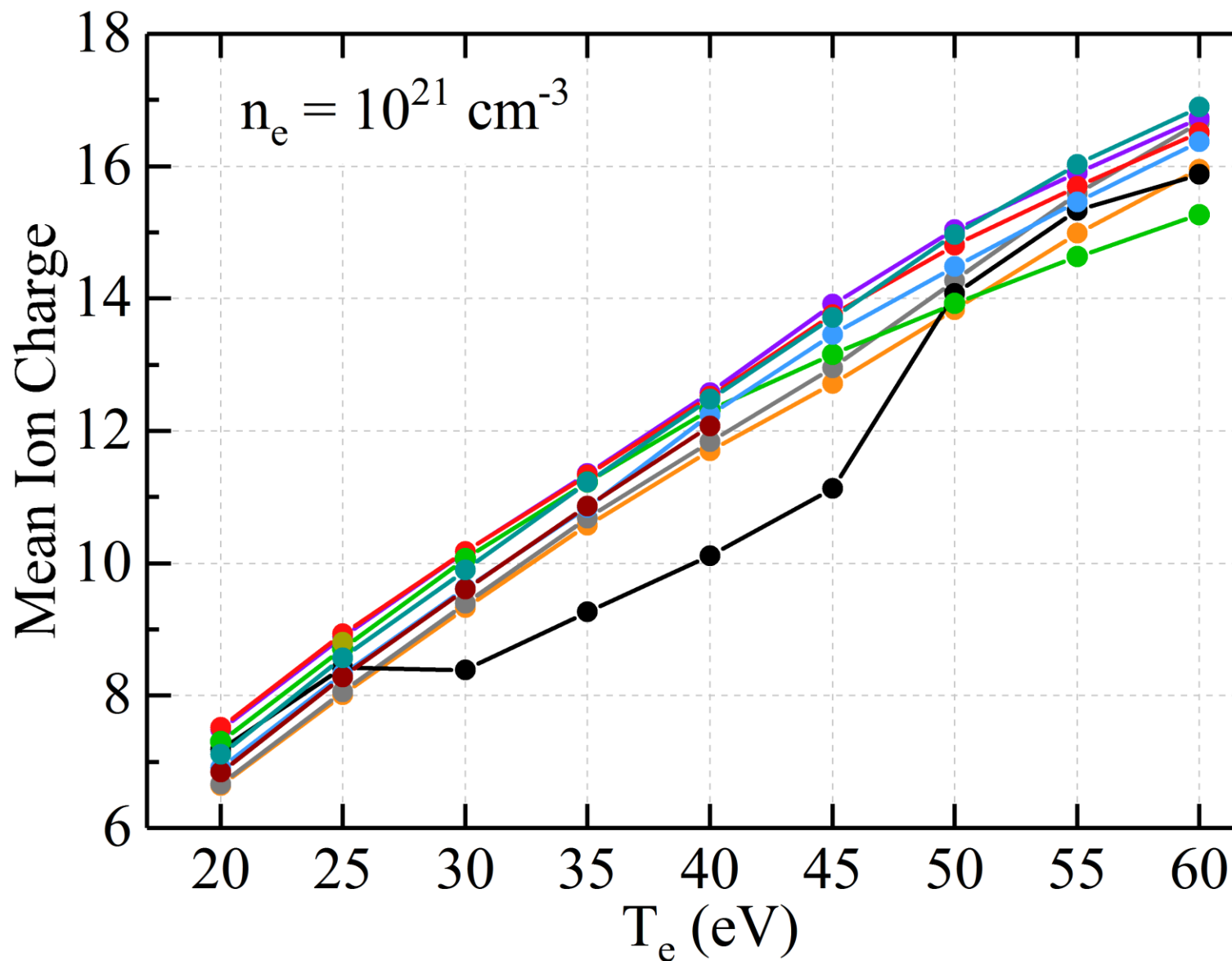


$$\text{Spectral purity} = \frac{\int_{13.365}^{13.635} \eta_\lambda d\lambda}{\int_5^{20} \eta_\lambda d\lambda}$$



$$n_e = 10^{21} \text{ cm}^{-3}$$

# $n_e = 10^{21} \text{ cm}^{-3}$ : Mean charge state



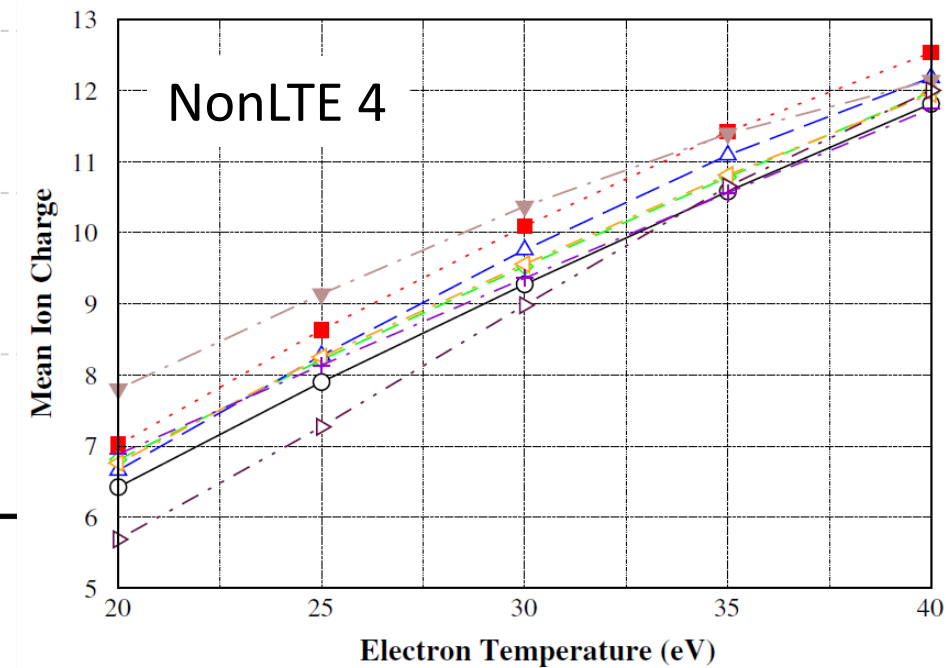
**Atomic structure**

$$\beta = 1.34 \times 10^{13} \frac{T_e^{7/2}}{n_e} \ll 1 \text{ for LTE conditions}$$

$4p^4$

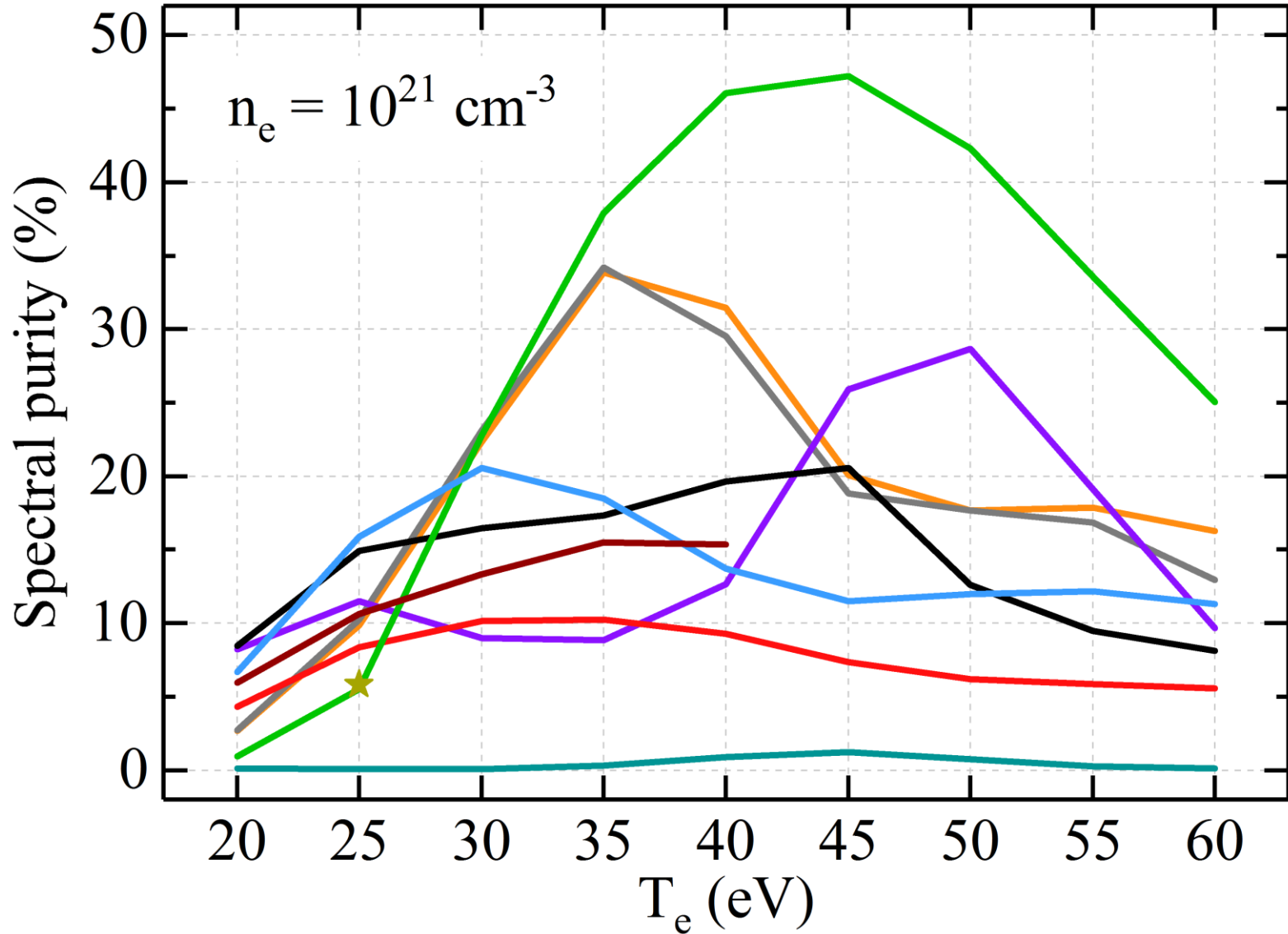
$$\beta \approx \mathbf{0.0005} \text{ for } T_e = 20 \text{ eV}$$

$$\beta \approx \mathbf{0.02} \text{ for } T_e = 60 \text{ eV}$$



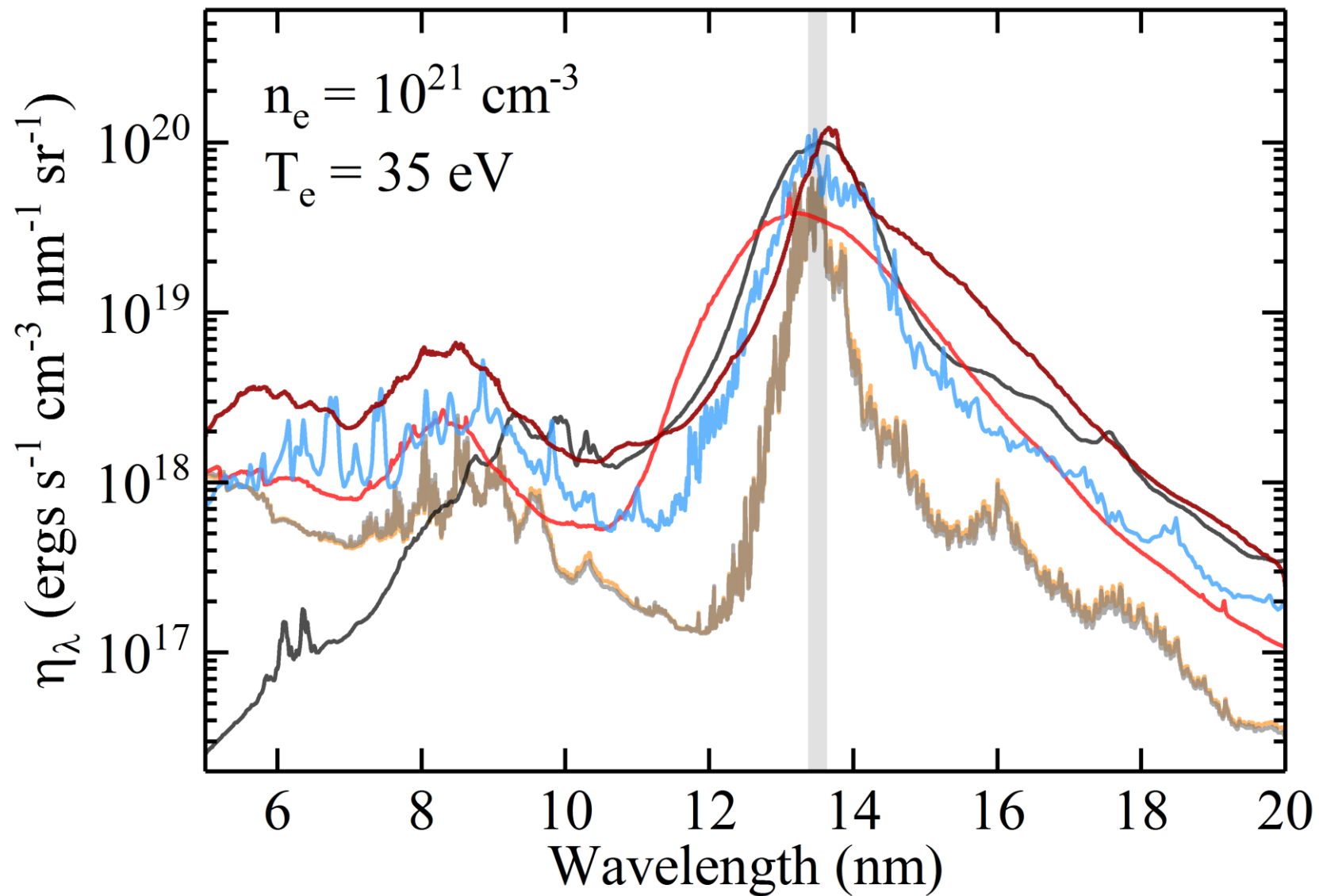


# $n_e = 10^{21} \text{ cm}^{-3}$ : Spectral purity

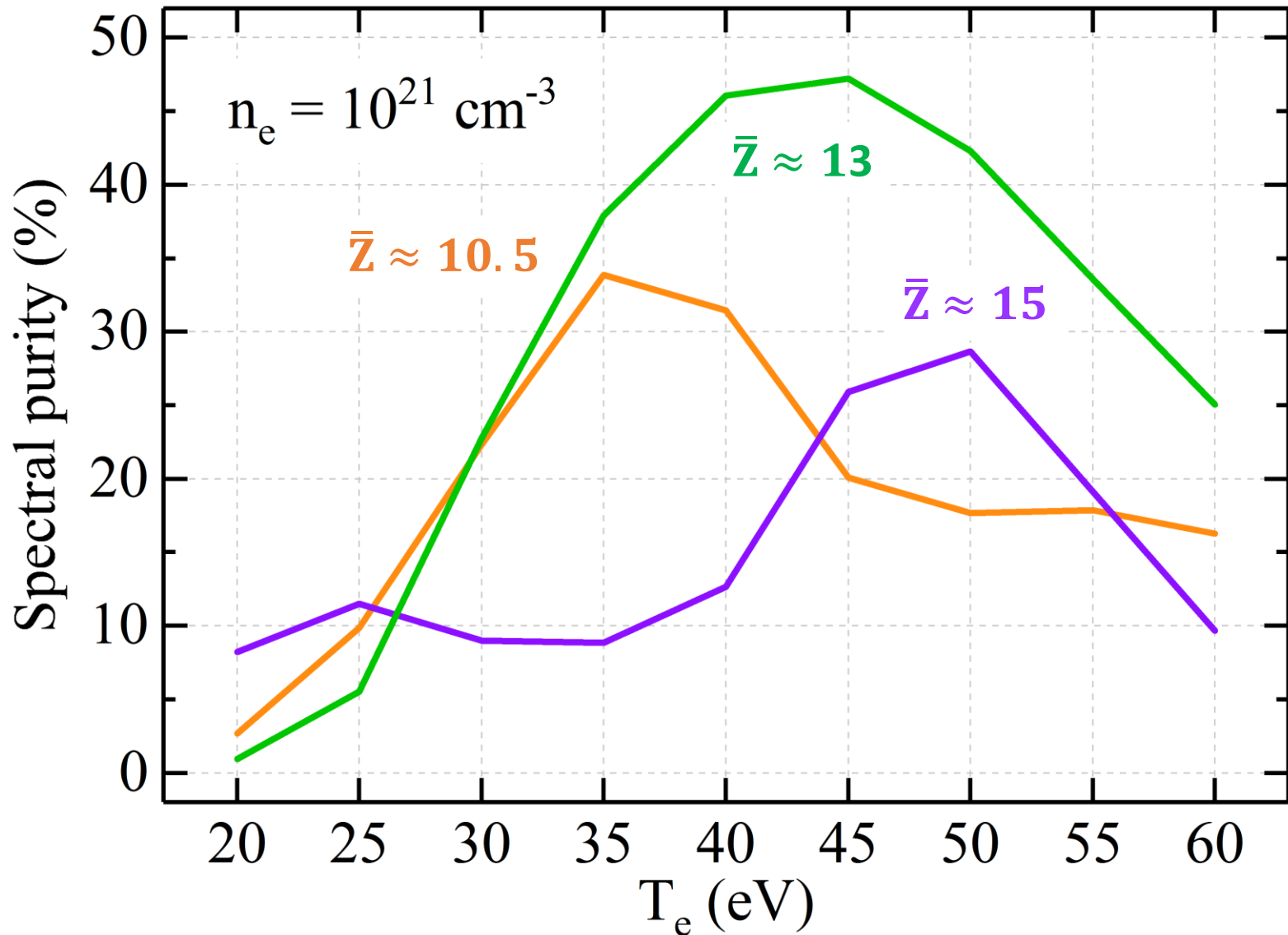


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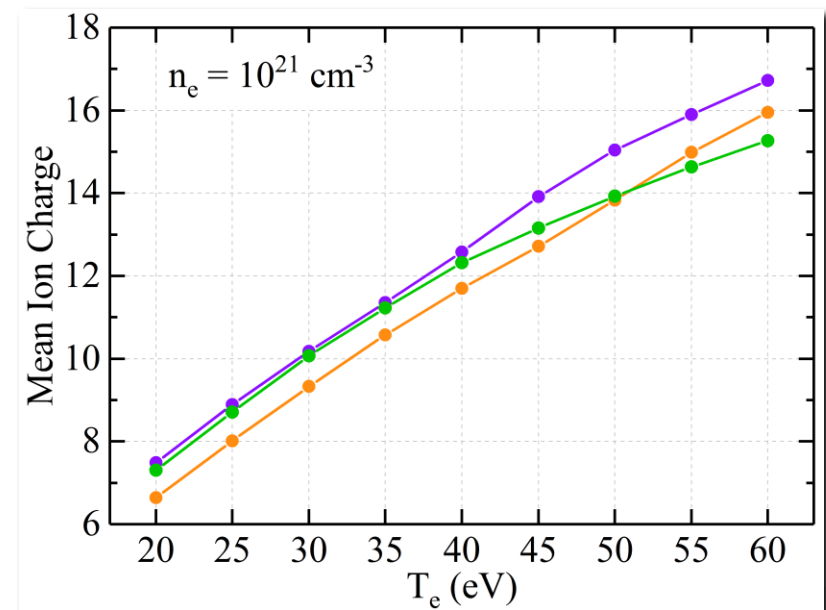
# $n_e = 10^{19} \text{ cm}^{-3}$ : Emissivity



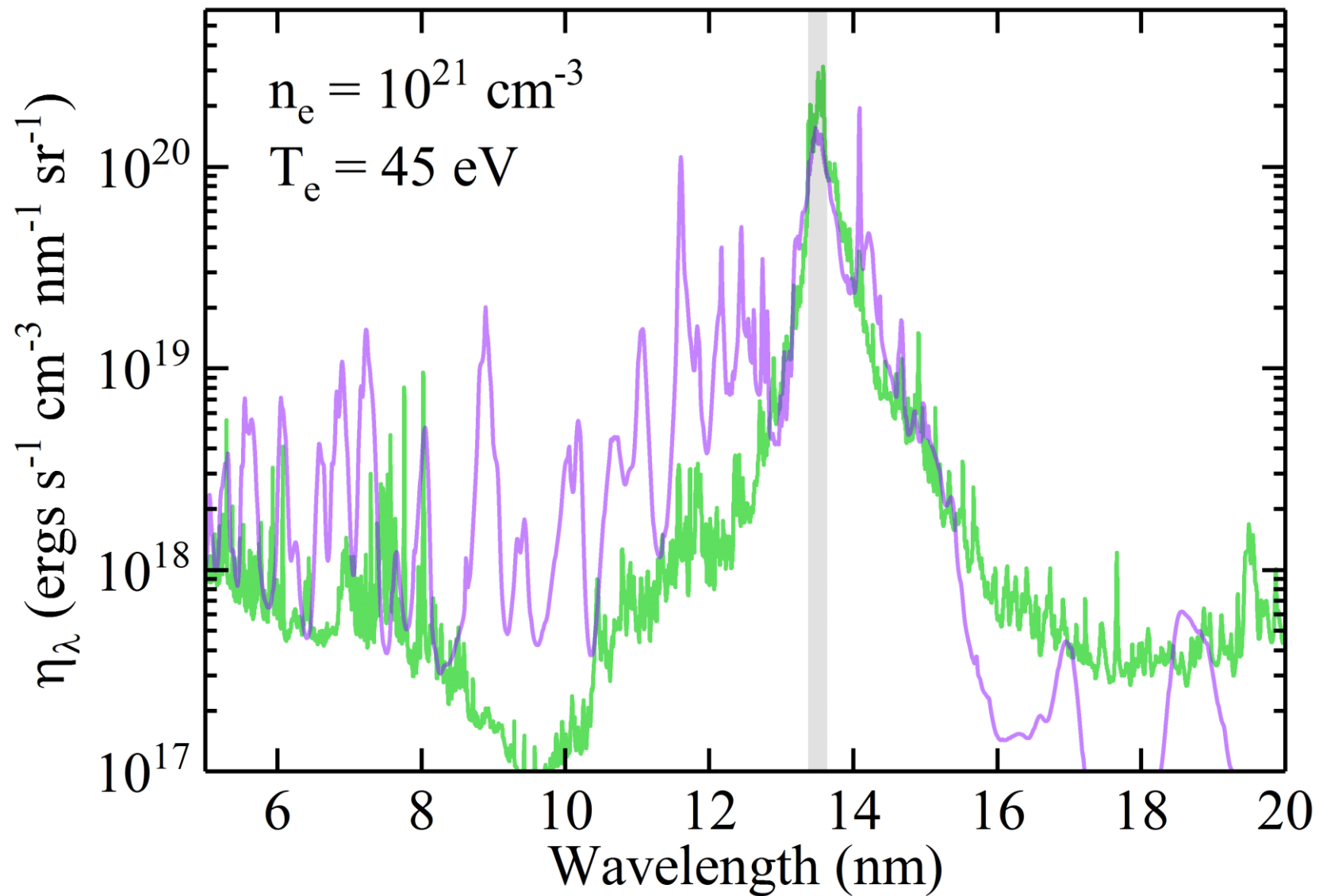
# $n_e = 10^{21} \text{ cm}^{-3}$ : Spectral purity



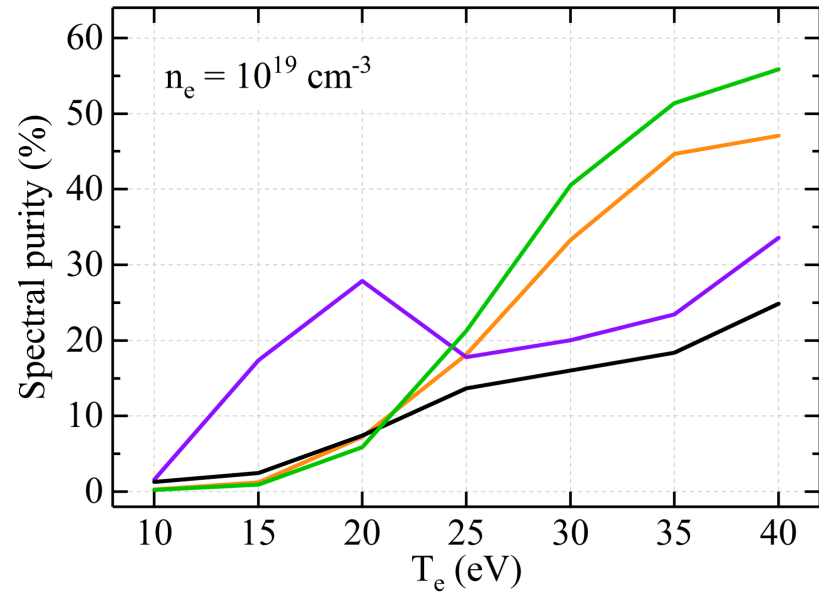
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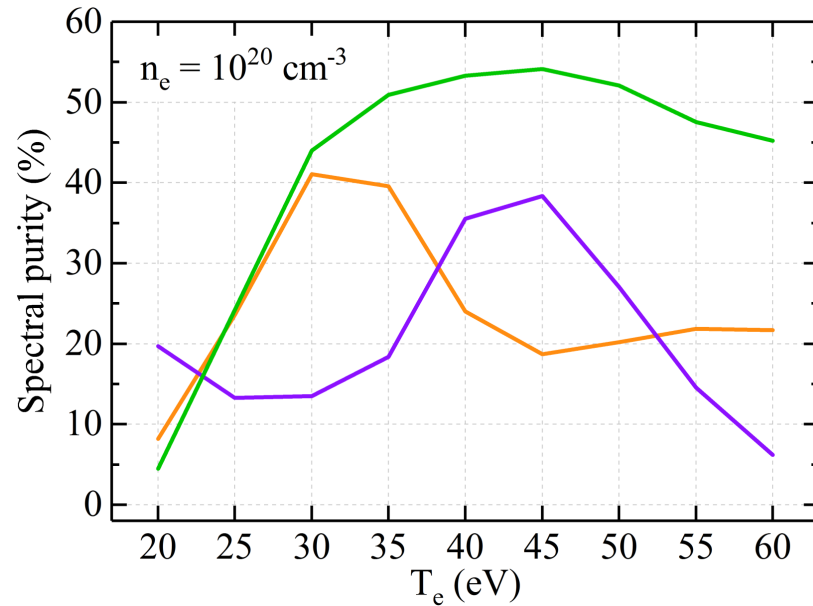
# $n_e = 10^{21} \text{ cm}^{-3}$ : Emissivity



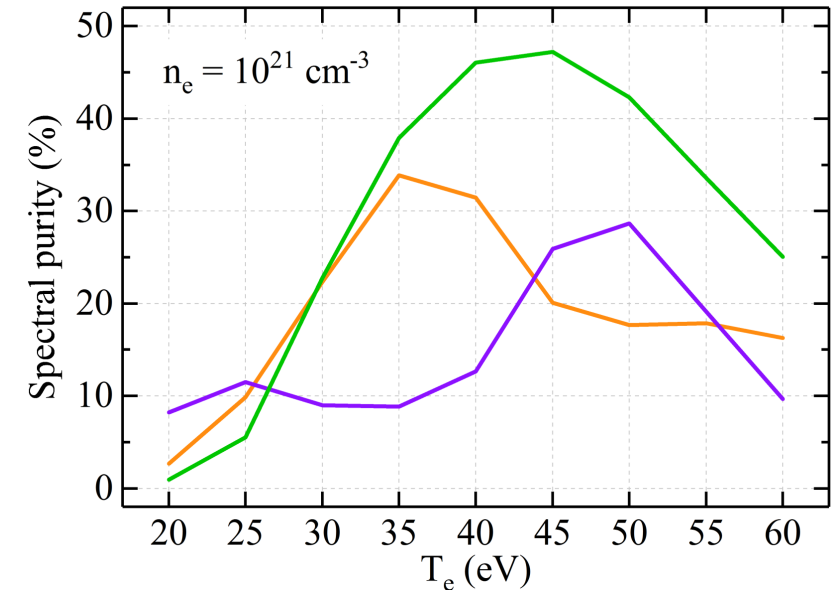
# Spectral purity: $n_e = 10^{19}$ , $10^{20}$ & $10^{21}$ cm<sup>-3</sup>



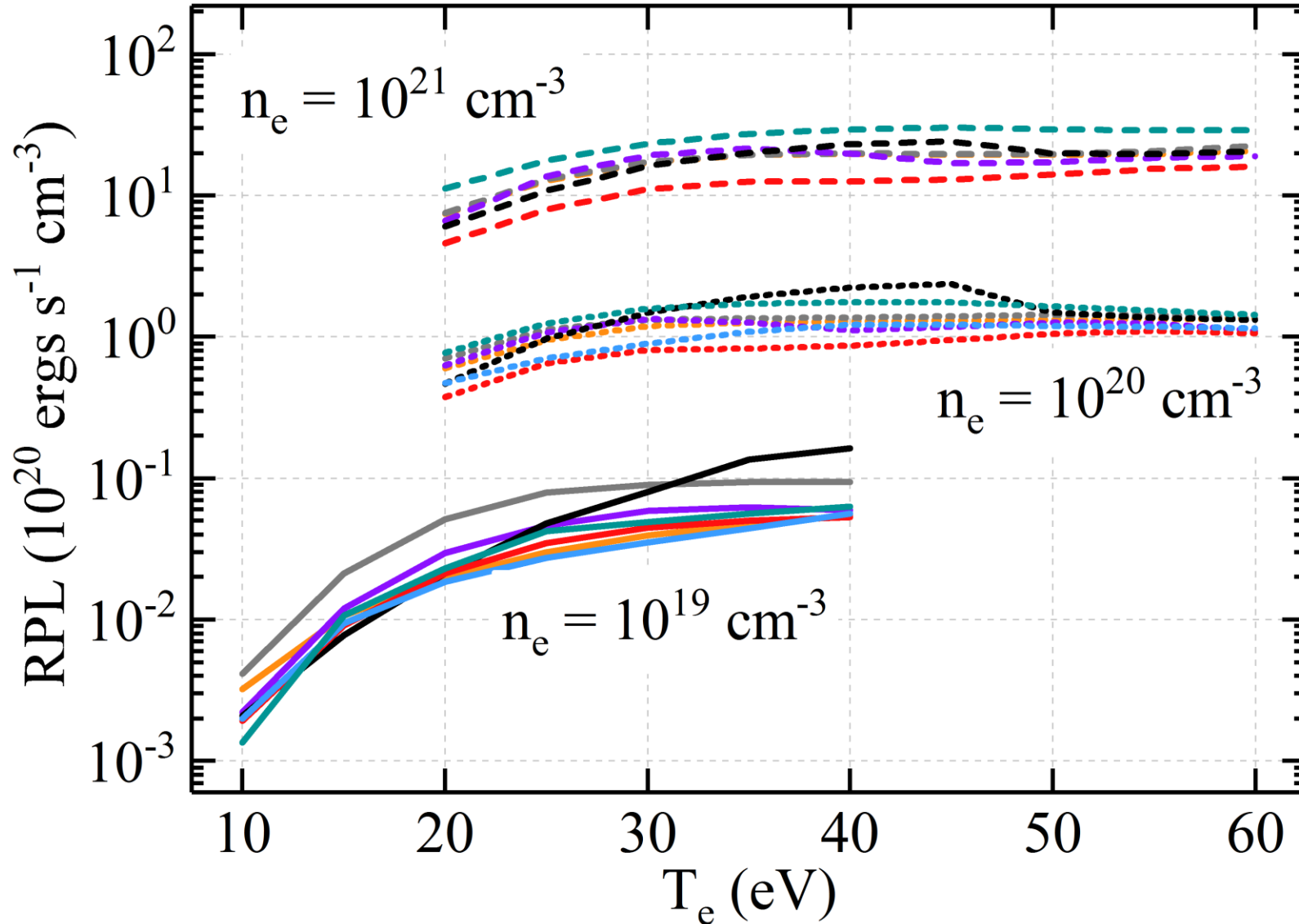
- Need higher temperatures at higher densities to achieve optimum charge state balance.



- Spectral purity decreases as you move to higher densities and higher temperatures



# Radiative power losses: $10^{19}$ , $10^{20}$ & $10^{21}$ $\text{cm}^{-3}$



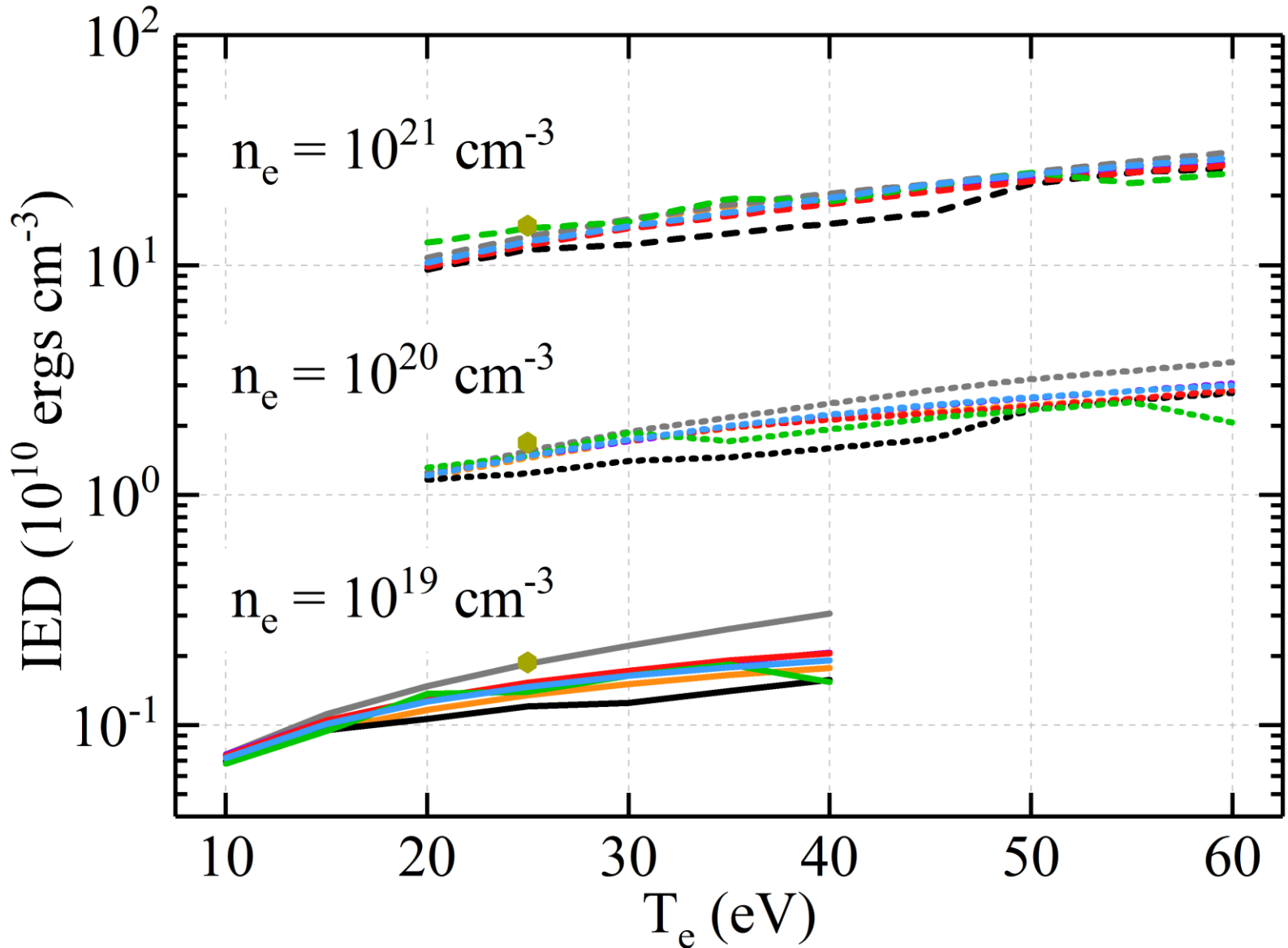
## Radiative Power Losses (RPL)

Total contribution from:

- **bound-bound**
- **bound-free** (recombin.) and
- **free-free transitions** (bremsstr.)

Good agreement between codes  
for all three electron density sets.

# Internal energy density: $10^{19}$ , $10^{20}$ & $10^{21}$ $\text{cm}^{-3}$



Energy level

Population density

$$\text{IED} = \sum_{i,Z} E_{i,Z} n_{i,Z}$$

levels, charge states

Good agreement between codes for all three electron density sets.

# Conclusion

- Best agreement between mean charge values at low  $T_e$ .
- LTE submissions predict highest spectral purity for  $\bar{Z} \approx \mathbf{12}$ . Greater spread in  $\bar{Z}$  for the non-LTE submissions.
- Spectral purity decreases with an increase in density (and temperature).
- Good agreement between codes for the radiative power losses and internal energy densities.