Ionization Cross Sections of Ions in Dense plasmas modified by the Transient Space Localization of Continuum Electrons

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Introduction

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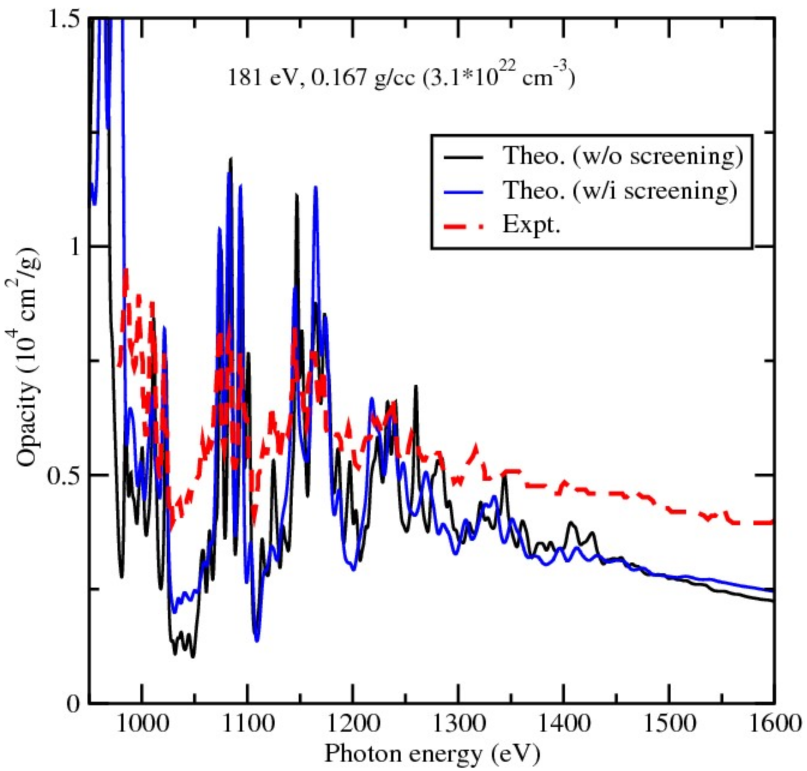
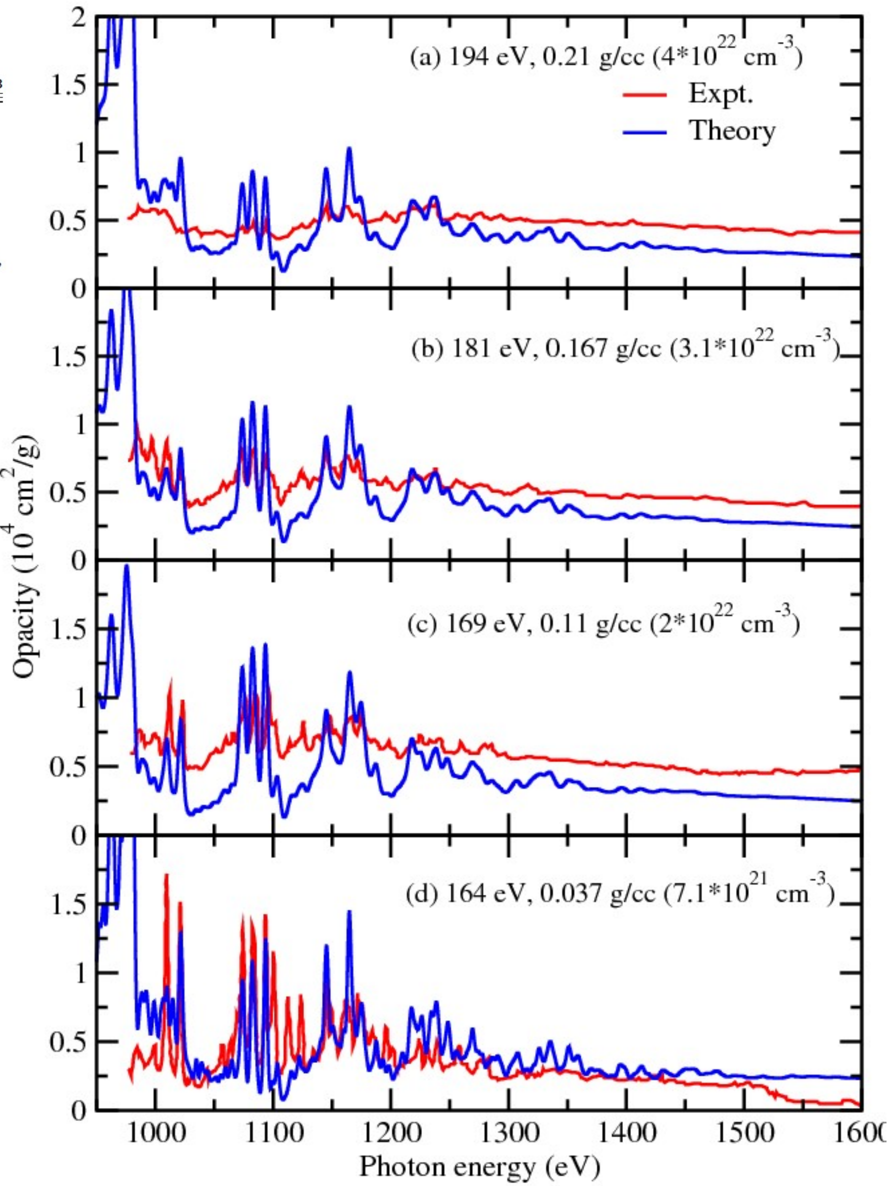
A higher-than-predicted measurement of iron opacity at solar interior temperatures

J. E. Bailey[1], T. Nagayama[1], G. P. Loisel[1], G. A. Rochau[1], C. Blancard[2], J. Colgan[3], Ph. Cosse[2], G. Faussurier[2], C. J. Fontes[3], F. Gilleron[2], I. Golovkin[4], S. B. Hansen[1], C. A. Iglesias[5], D. P. Kilcrease[3], J. J. MacFarlane[4], R. C. Mancini[6], S. N. Nahar[7], C. Orban[7], J.-C. Pain[2], A. K. Pradhan[7], M. Sherrill[3] & B. G. Wilson[5]



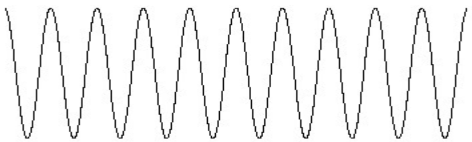


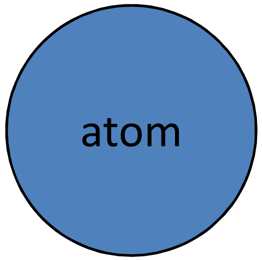
Introduction

Mean free path: $\bar{l} = \frac{\upsilon}{\nu}$

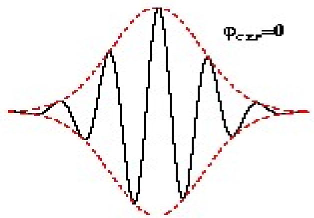
$P_{\varepsilon l}$ is the radius wave function of free electron and is renormalized.

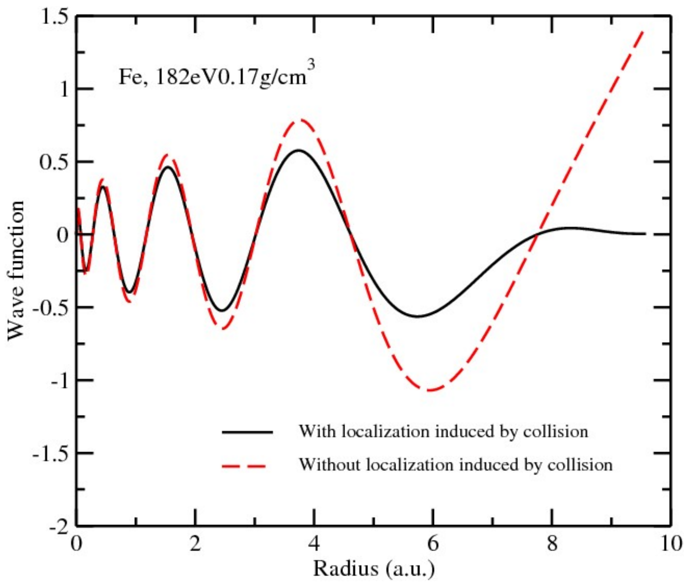
In free space





In plasma





$$P_{\varepsilon l}(r) = P_{\varepsilon l}^{old}(r)\exp\left(-\frac{r}{\bar{l}}\right)$$

$$p_{ij} \propto \left|\left\langle \Psi_i \left| \hat{T} \right| \Psi_j \right\rangle\right|^2$$

Opacity with Debye like screening

$$\boxed{K_\nu = \frac{N_A}{A}\left[\sigma^{bb}(h\nu)+\sigma^{bf}(h\nu)+\sigma^{ff}(h\nu)\right]\times(1-e^{-h\nu/kT})+K_{sc}}$$

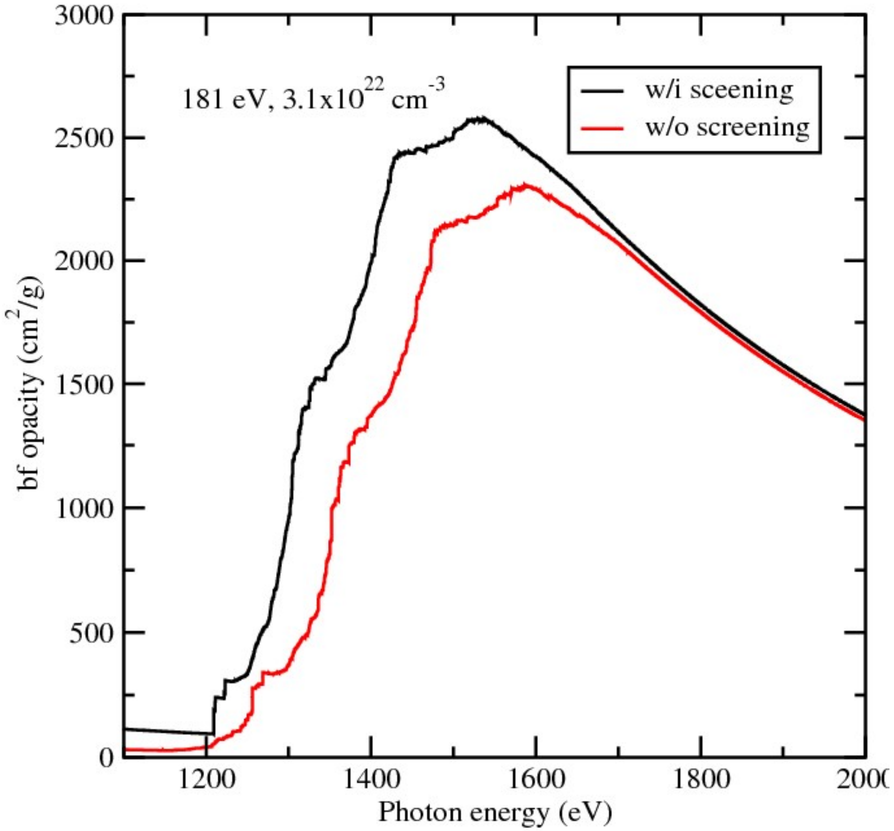
$$\hat{H} = \sum_i [c\vec{\alpha}\cdot\vec{p}+\beta mc^2-\frac{Z}{r_i}]+\sum_{i>j}\frac{1}{r_{ij}}+\sum_i \phi_f(r_i)$$

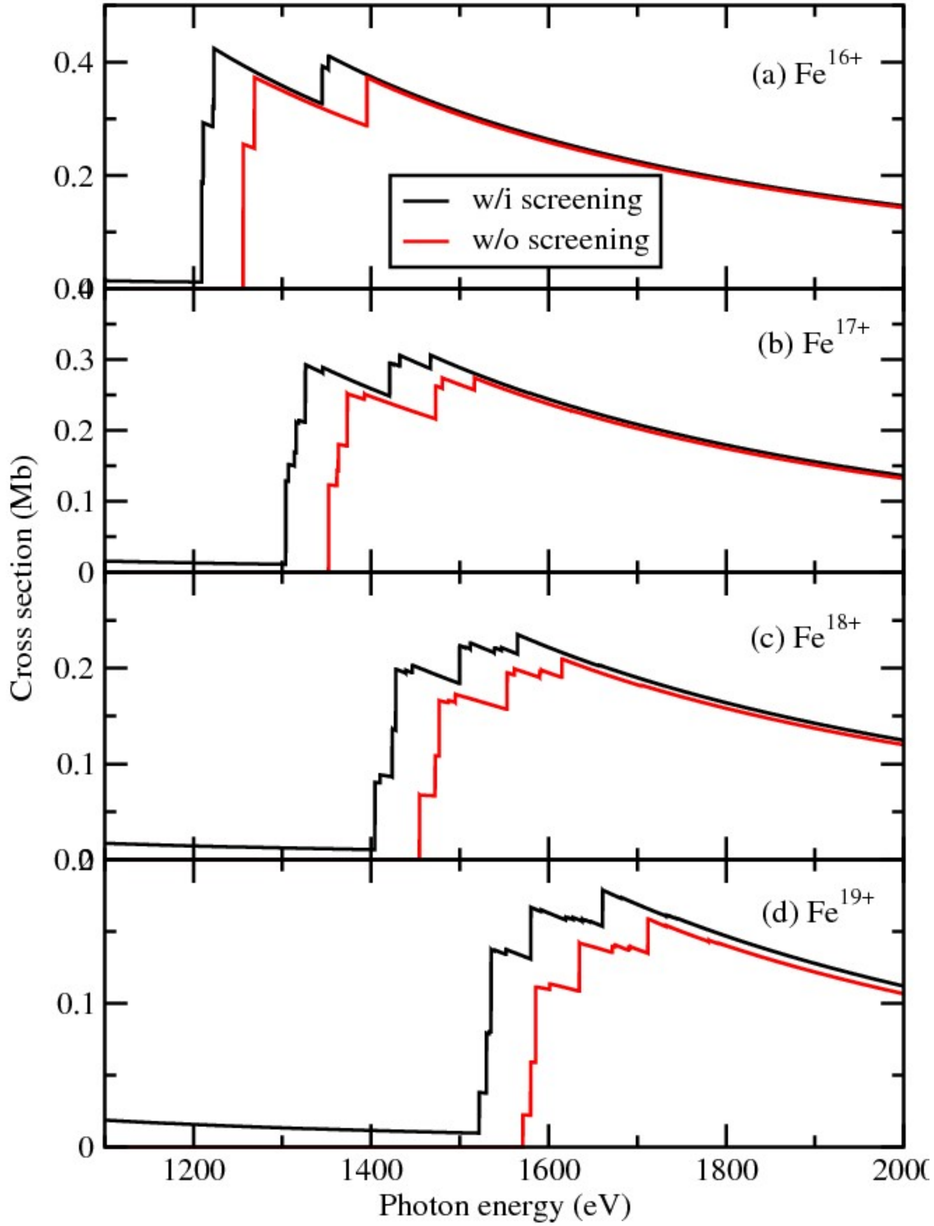
$$\phi_f(r_i) = 4\pi\left[\frac{1}{r_i}\int_0^{r_i} r_1 + \int_{r_i}^{R_0} \right] r_1\rho_f(r_1)dr_1$$

$$\rho_f(r) = \frac{1}{\pi^2}\int_{p_0(r)}^{+\infty}\frac{p^2dp}{\exp\left(\frac{\sqrt{p^2c^2+c^4}-c^2-U(r)-\mu}{k_BT}\right)+1}$$

$2s^22p^63s$, $2s^22p^53s$, $2s^22p^43s$

Opacity with Debye like screening





Finite quantum coherence length for the thermal continuum electrons

LORENTZIAN PROFILE

When the radial wave functions are assumed to be plane waves, where $P_{\epsilon\kappa}(r) = \sqrt{\frac{2}{\pi k}} exp(ikr)$, the superimposed radial wave function

$$\mu_{\epsilon_0\kappa}(r) = \frac{1}{\sqrt{2\pi}} \int_0^\infty F(k) \sqrt{\frac{2}{\pi k}} exp(ikr) dk \tag{1}$$

When $\Delta k \ll k$, $\sqrt{\frac{2}{\pi k}} = \sqrt{\frac{2}{\pi k_0}}$

$$\begin{aligned} \mu_{\epsilon_0\kappa}(r) &= \frac{1}{\pi\sqrt{k_0}} \int_0^\infty F(k) exp(ikr) dk \\ &= \frac{1}{\pi\sqrt{k_0}} \int_0^\infty \frac{1}{k - k_0 - i\Delta k} exp(ikr) dk \\ &= \frac{1}{\pi\sqrt{k_0}} exp(ik_0 r) exp(-\Delta k r) \end{aligned} \tag{2}$$

Where Δk is the half width at half maximun of k.

The normalized radial wave function

$$\mu_{\epsilon_0\kappa}(r) = \frac{2k_0\sqrt{\Delta k}}{\sqrt{k_0^2 - \Delta k^2}} exp(ik_0 r) exp(-\Delta k r) \tag{3}$$

$$\Delta k' = \int P_{cm}(1 - cos\theta)(\frac{d\sigma}{d\Omega})_{cm} d\Omega \tag{4}$$

Finite quantum coherence length for the thermal continuum electrons

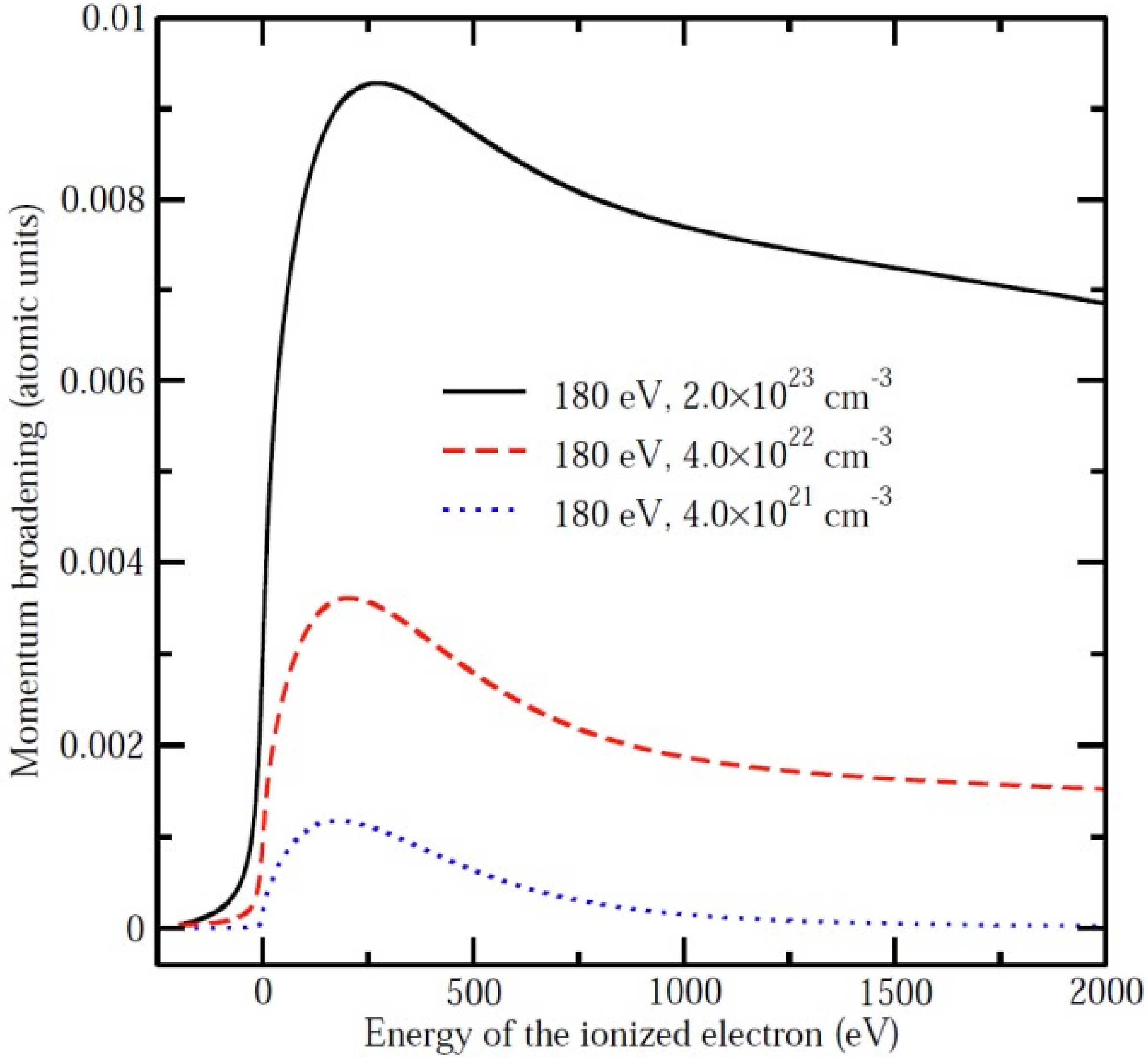


FIG. 1. Momentum broadening of the ionized electron. The ionized electron is ejected from a photoionization process of Fe^{16+} embedded in iron plasmas at a temperature of 180.0 eV and electron densities of 4.0×10^{21}, 4.0×10^{22}, and 2.0×10^{23} cm^{-3}. Atomic units have been used for the HWHM of the momentum broadening.

Finite quantum coherence length for the thermal continuum electrons

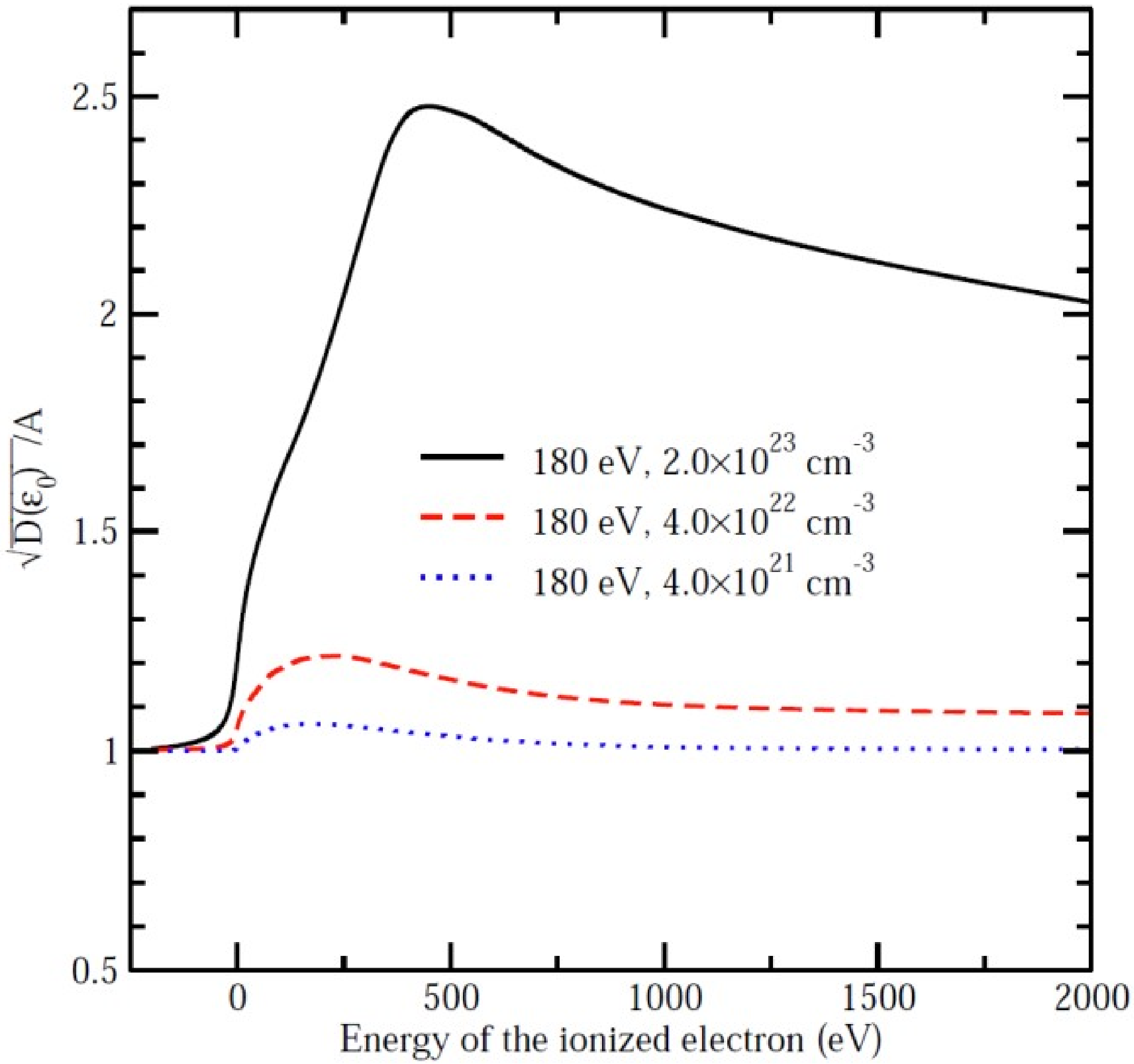


FIG. 3. Normalized DOS of the ionized electron. Shown are the ratios of the square root of DOS to the normalization constant A (see Methods) of the continuum wavefunction in the photoionization process of $h\nu + 1s^22s^22p^6\ ^1S \rightarrow 1s^22s^22p^5\ ^2P^o + e(\epsilon_0 s)$ of Fe^{16+} embedded in the same plasma conditions as in Fig. 1.

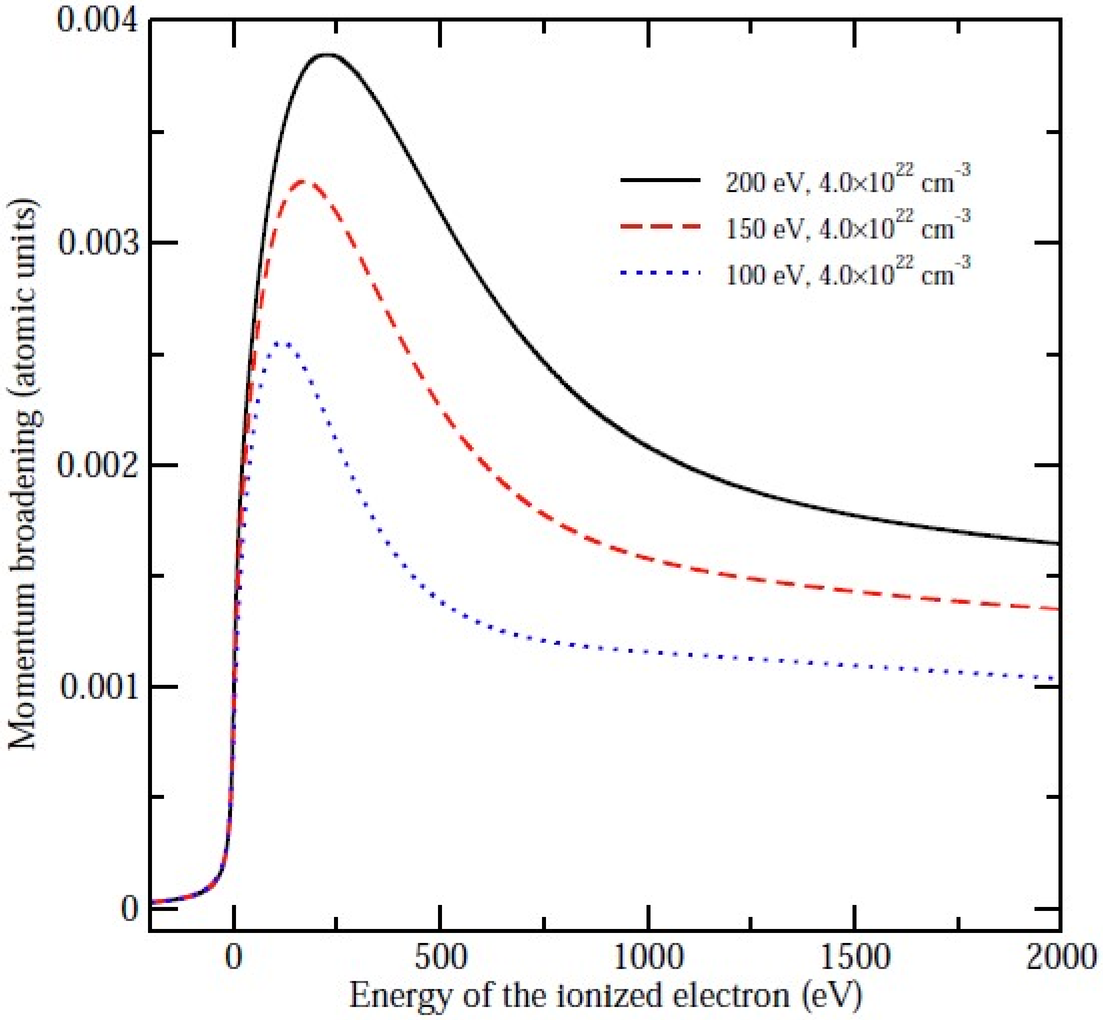


图 4.2　动量展宽随等离子体温度的变化。连续电子是电子密度为 4.0×10^{22}，温度为 100, 150, 200 eV 条件下铁等离子体 Fe^{16+} 基态光电离发射出的连续电子。动量展宽的半高半宽使用的是原子单位。

Finite quantum coherence length for the thermal continuum electrons

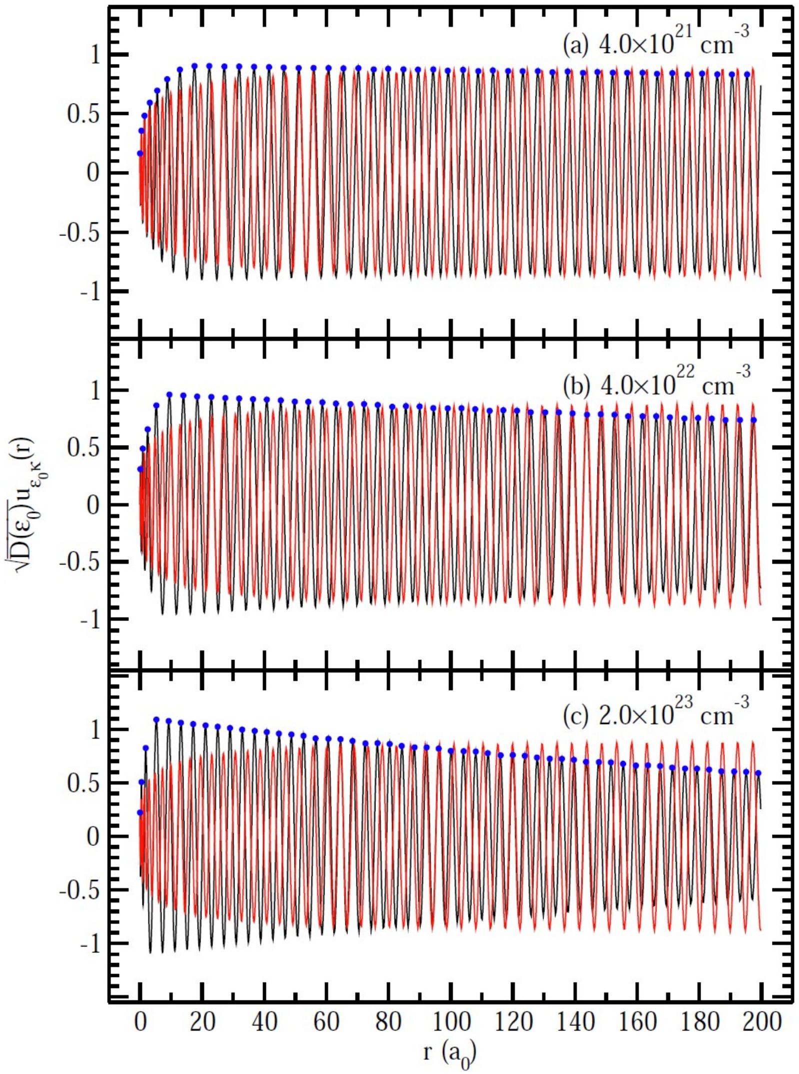


FIG. 2. Radial wavefunction of the ionized electron. The ionized electron is ejected from the photoionization process of $h\nu + 1s^2 2s^2 2p^6\ ^1S \rightarrow 1s^2 2s^2 2p^5\ ^2P^o + e(\epsilon_0 s)$ of Fe^{16+} with a central kinetic energy ϵ_0 of 20.0 eV and is immersed in the same plasma conditions as in Fig. 1. The envelop line denoted by solid dots is given to guide the eyes. To have a comparison with the free ion, the wavefunction has been multiplied by the square root of DOS.

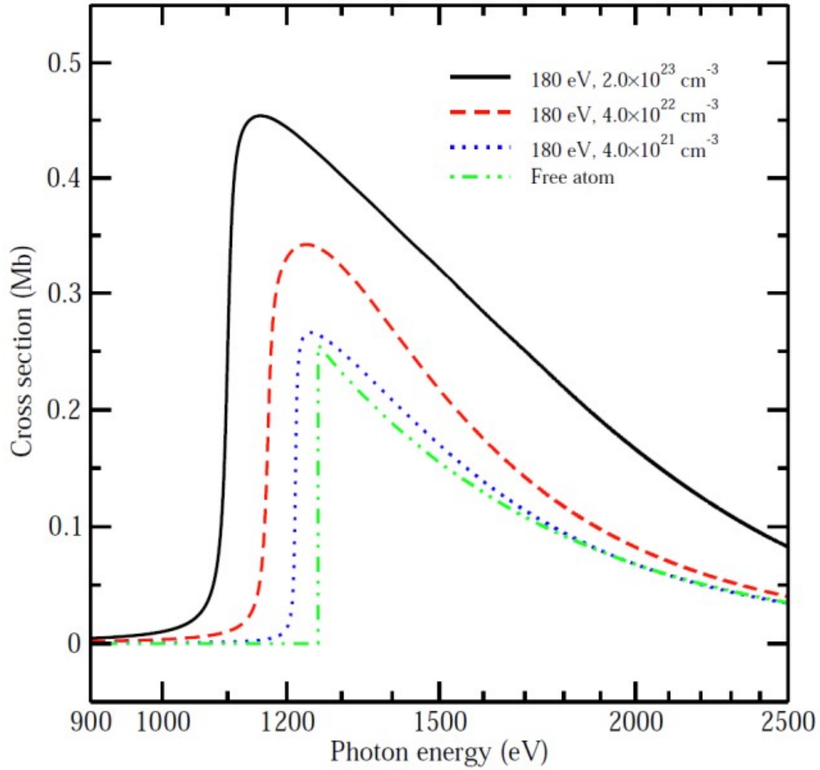


FIG. 4. Enhanced photoionization processes embedded in dense plasmas. The direct photoionization cross section of $h\nu + 1s^2 2s^2 2p^6\ ^1S \rightarrow 1s^2 2s^2 2p^5\ ^2P^o$ +e of Fe^{16+} is compared with that of the free ion. The plasma conditions are assumed the same as in Fig. 1.

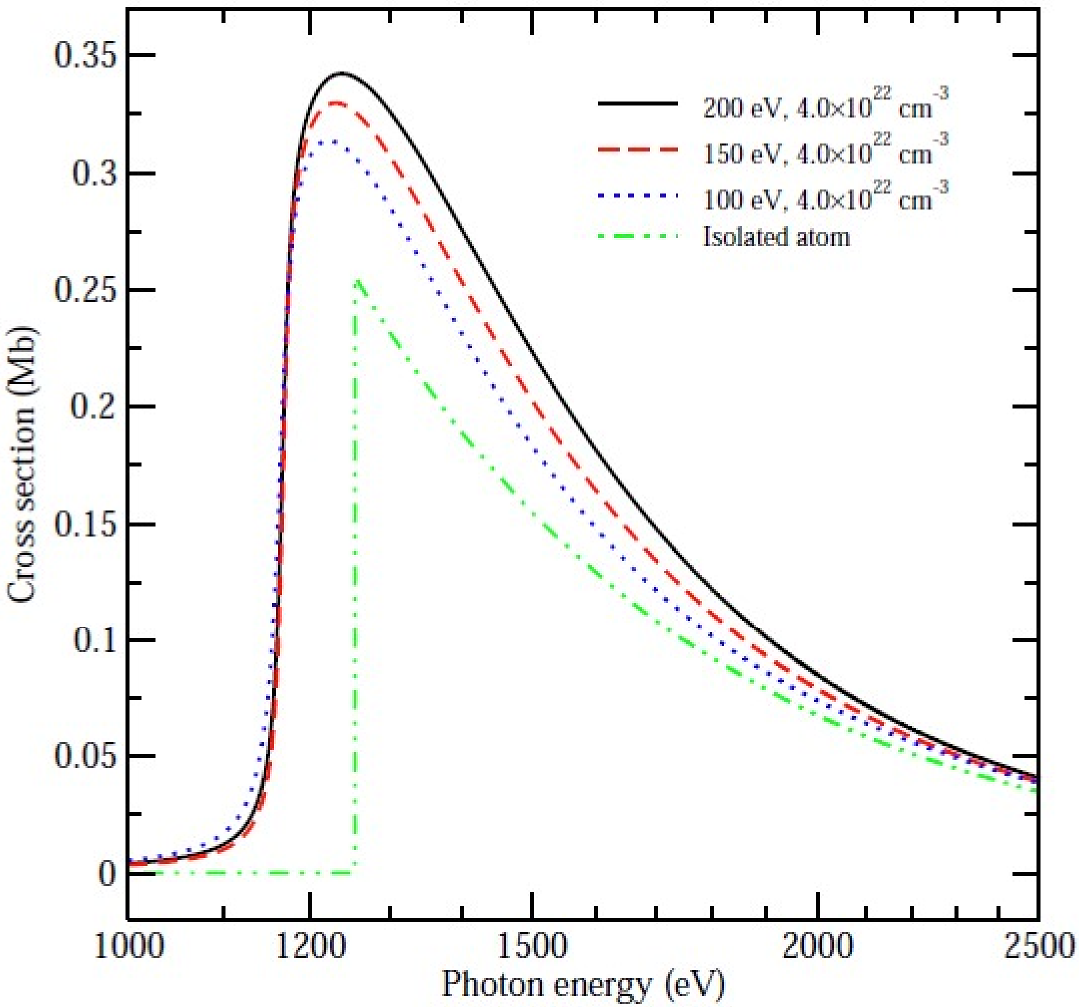


图 4.6　温度对光电离截面增强效应的影响。图中给出的是铁等离子体的 Fe^{16+} $h\nu + 1s^2 2s^2 2p^6\ {}^1S \rightarrow 1s^2 2s^2 2p^5\ {}^2P^o + e$ 的直接光电离截面。黑色实线、红色虚线和蓝色点线代表的是电子密度为 4.0×10^{22} cm^{-3}，温度为 200，150,100 eV 的光电离截面，绿色点虚线代表的是孤立原子的光电离截面。

Finite quantum coherence length for the thermal continuum electrons

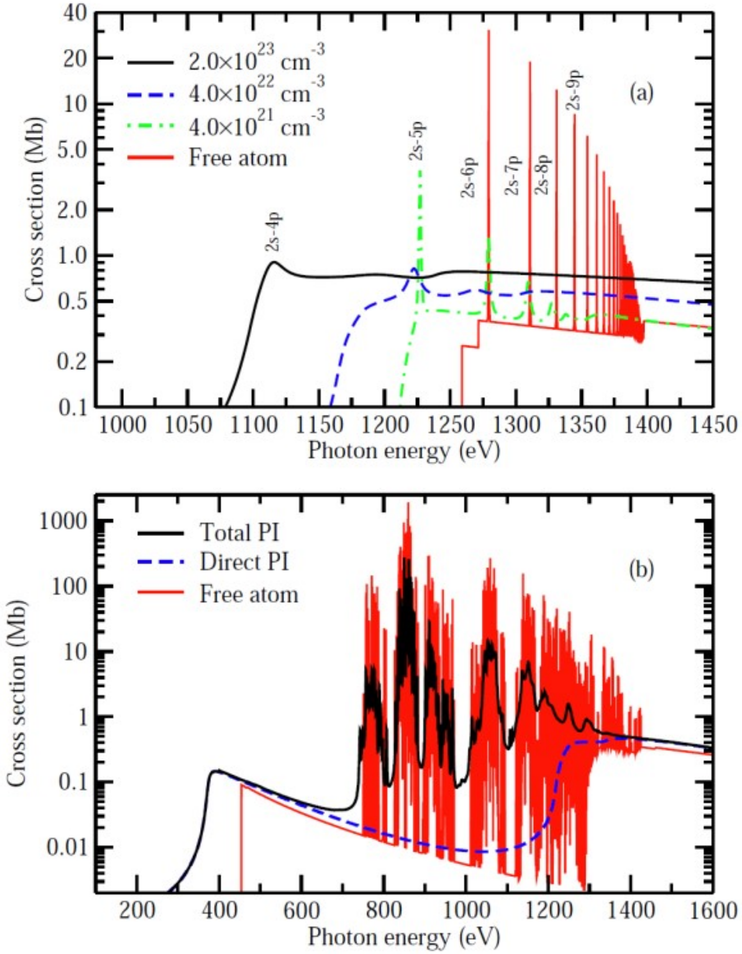
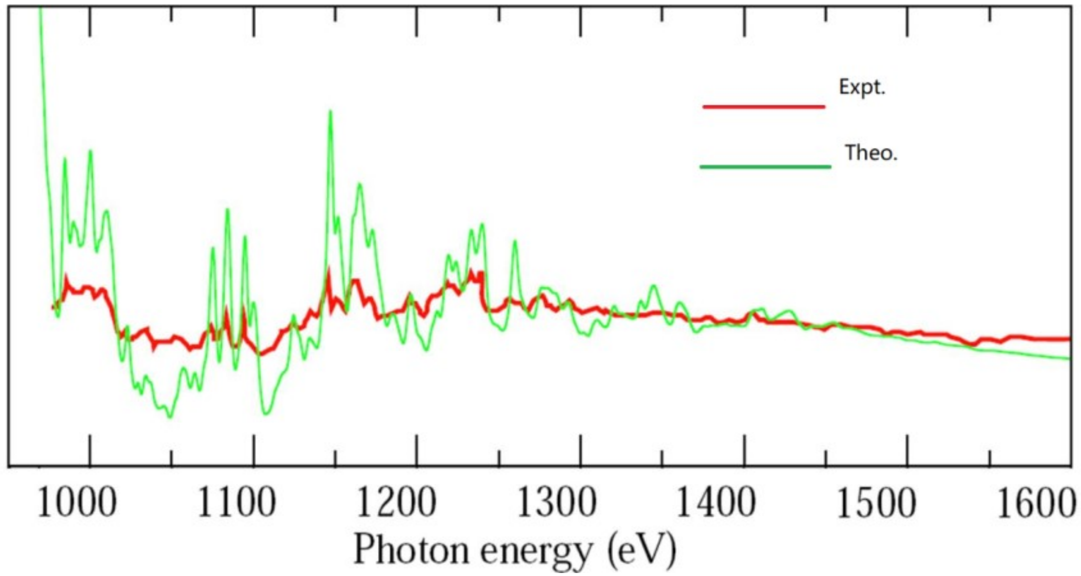
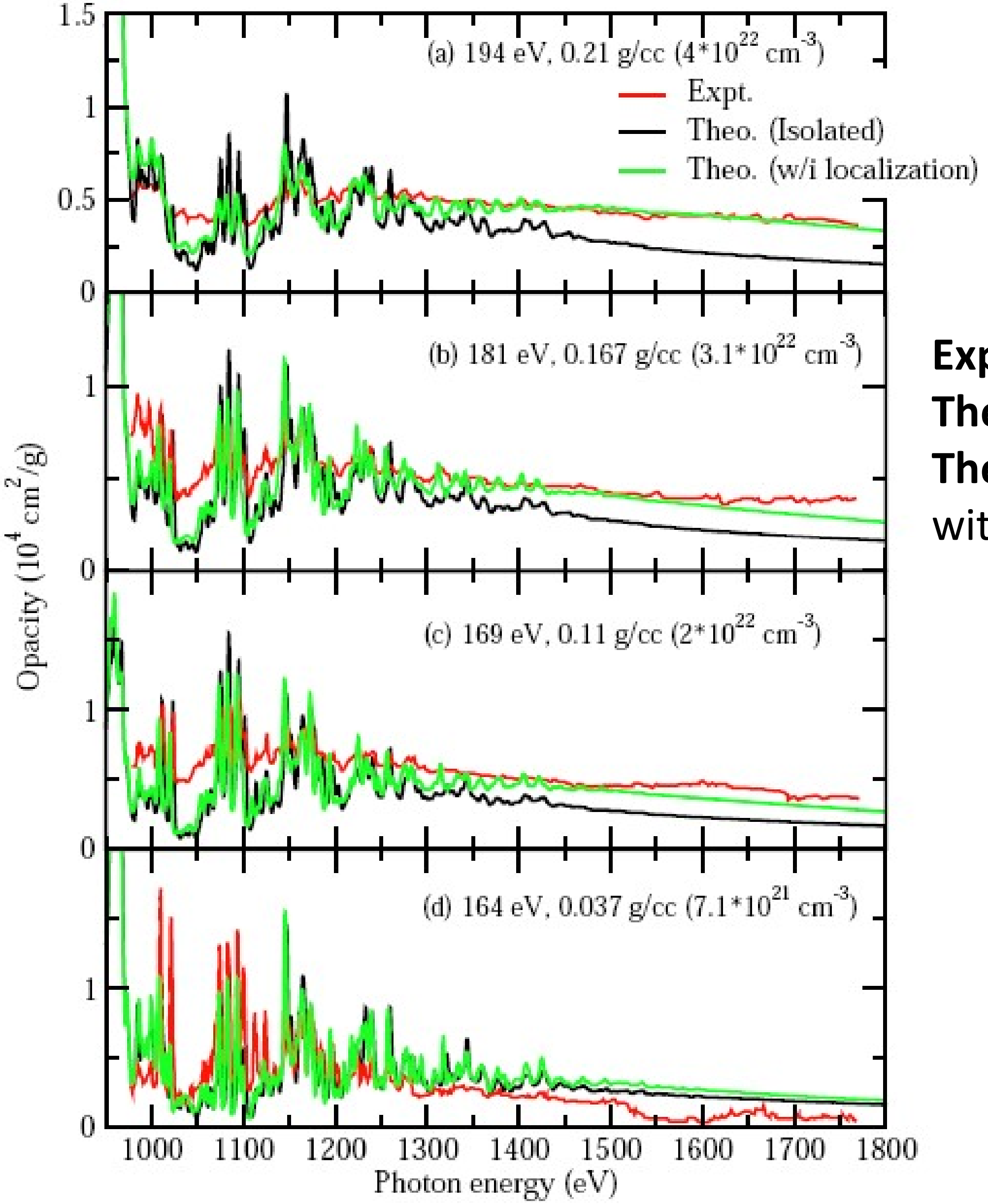


FIG. 5. Total photoionization cross sections. (a) For the ground level $1s^2 2s^2 2p^6\ ^1S$ of Fe^{16+} including both direct ionization of $2p$ and $2s$ electrons and indirect resonant processes at the same plasma environments as in Fig. 1. (b) For the excited state $1s^2 2s^2 2p^5 3d\ ^1P^o$ of Fe^{16+}, which is assumed to be embedded in an iron plasma at an electron density of 3.0×10^{22} cm^{-3} and a temperature of 180.0 eV.



Te=194 eV, $n_e=4\times10^{22}$ /cm^3

Comparison with experiment using CSD by Saha equation



Expt.: J. Bailey et al.. Nature 517, 56 (2015).
Theo. (Isolated): using free-atom data
Theo. (w/i localization): using atomic data with electron localization effect

Nuclear thermal motion driven electronic states

Quantum Molecular Dynamics

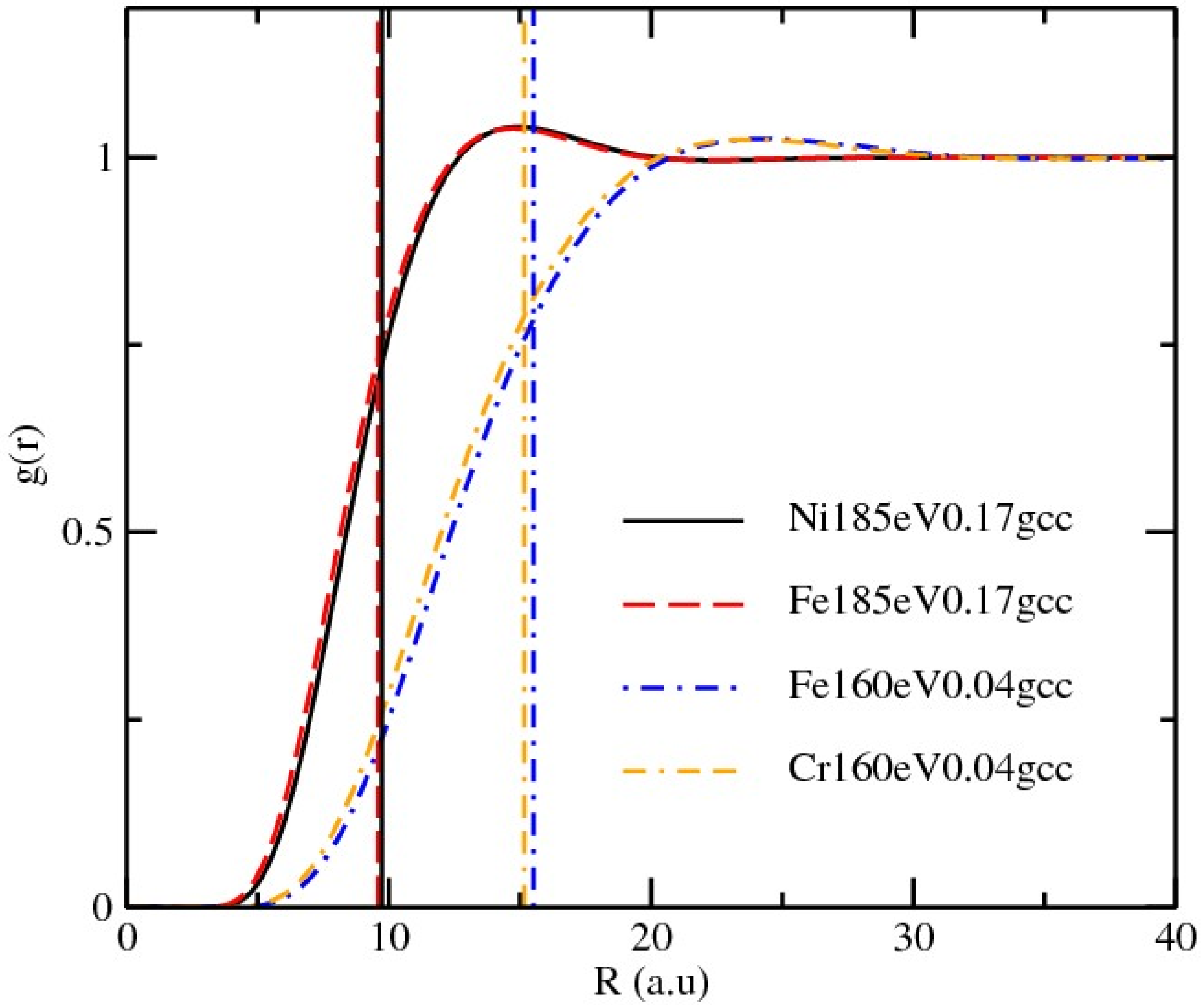
- **QMD:**
  - Electronic states are described by using DFT
  - ions' moving on smooth potential surface is described by Newton's equation
- **Langevin molecular dynamics in condensed matter and material sciences**
  - ions in Langevin equation

$$M_I \ddot{\mathbf{R}}_I = \mathbf{F} - \gamma_t M_I \dot{\mathbf{R}}_I + \mathbf{N}_I$$

γ_t **represents the contribution of thermostat for controlling the temperature of the system.**

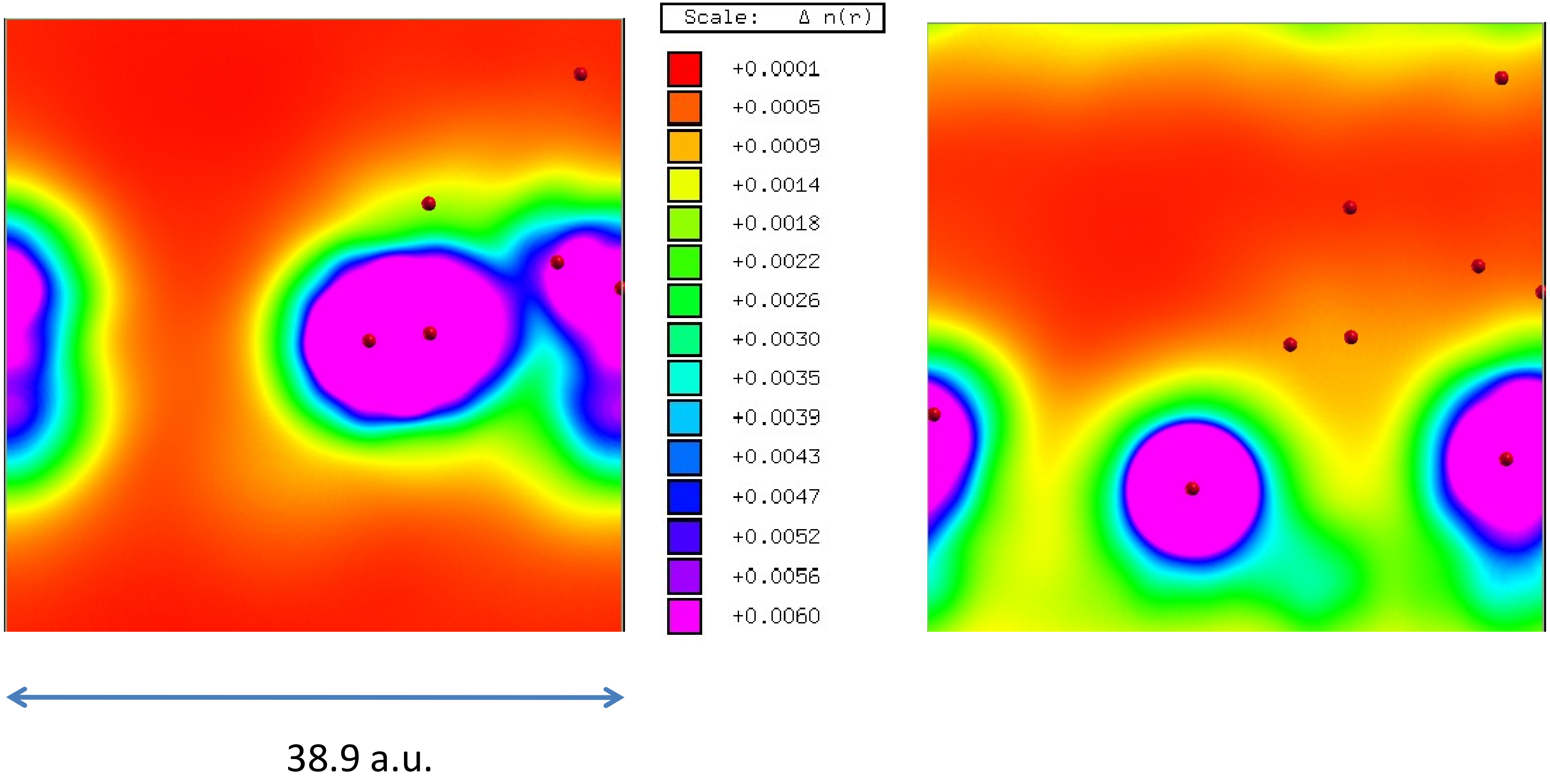
Nuclear thermal motion driven electronic states

Simulation for Sandia's experimental plasma conditions

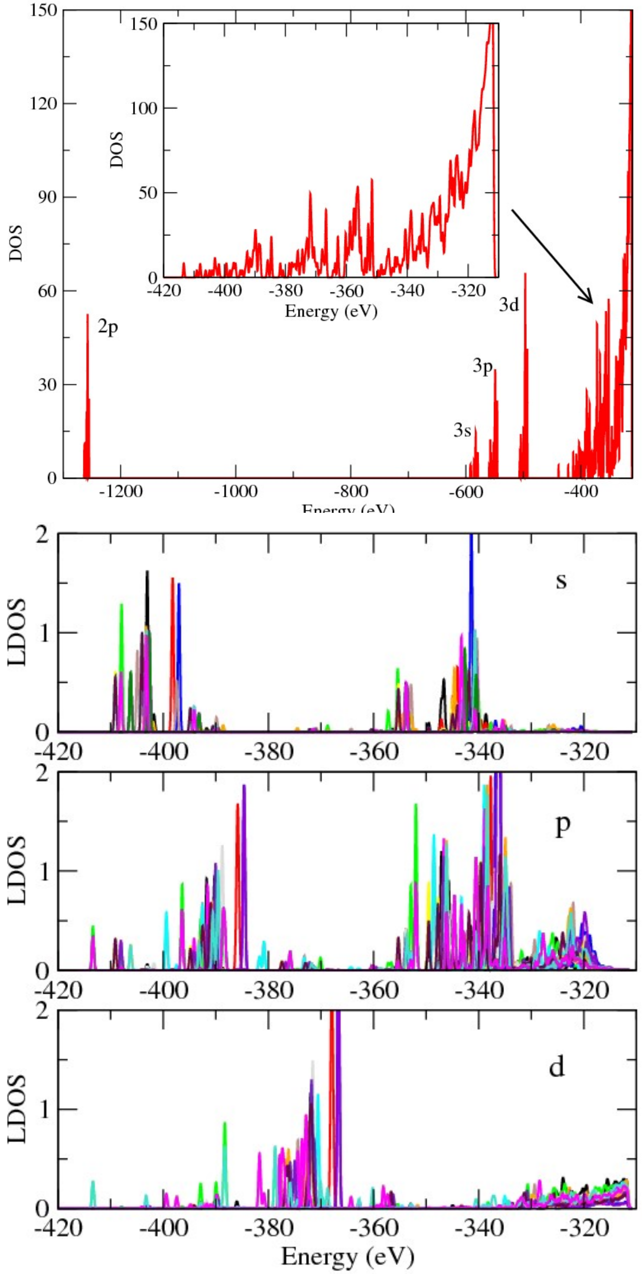


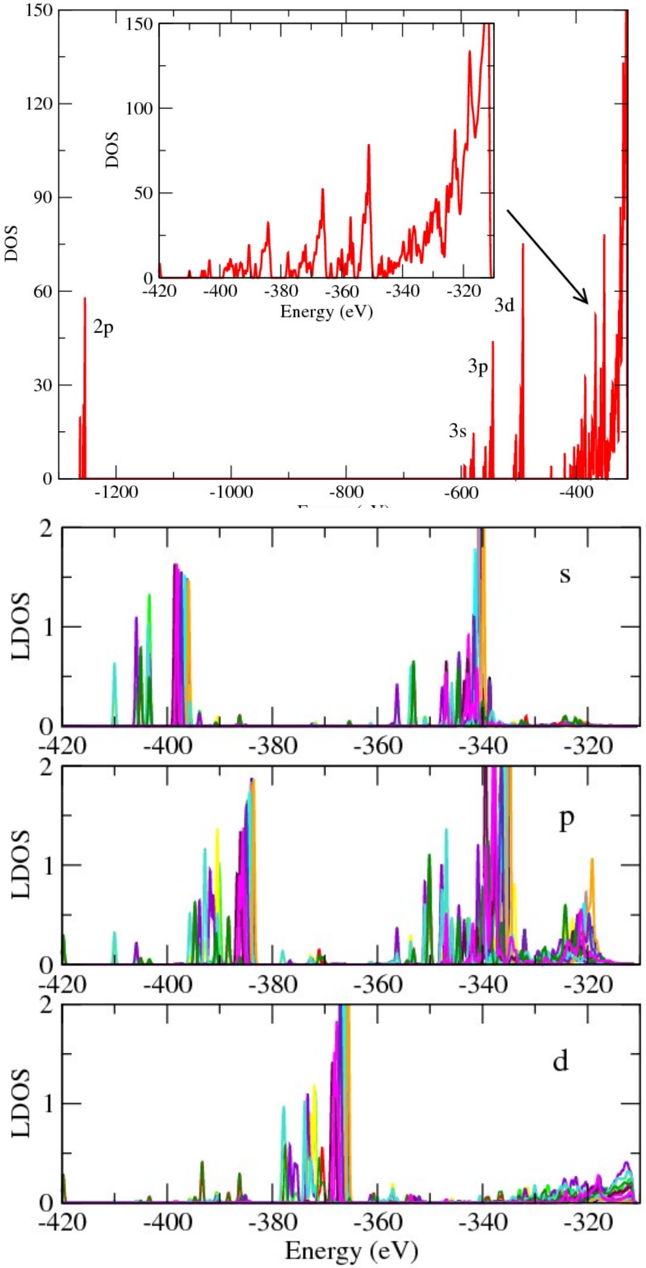
Nuclear thermal motion driven electronic states

The electron density distribution around the ions in the cell



Nuclear thermal motion driven electronic states

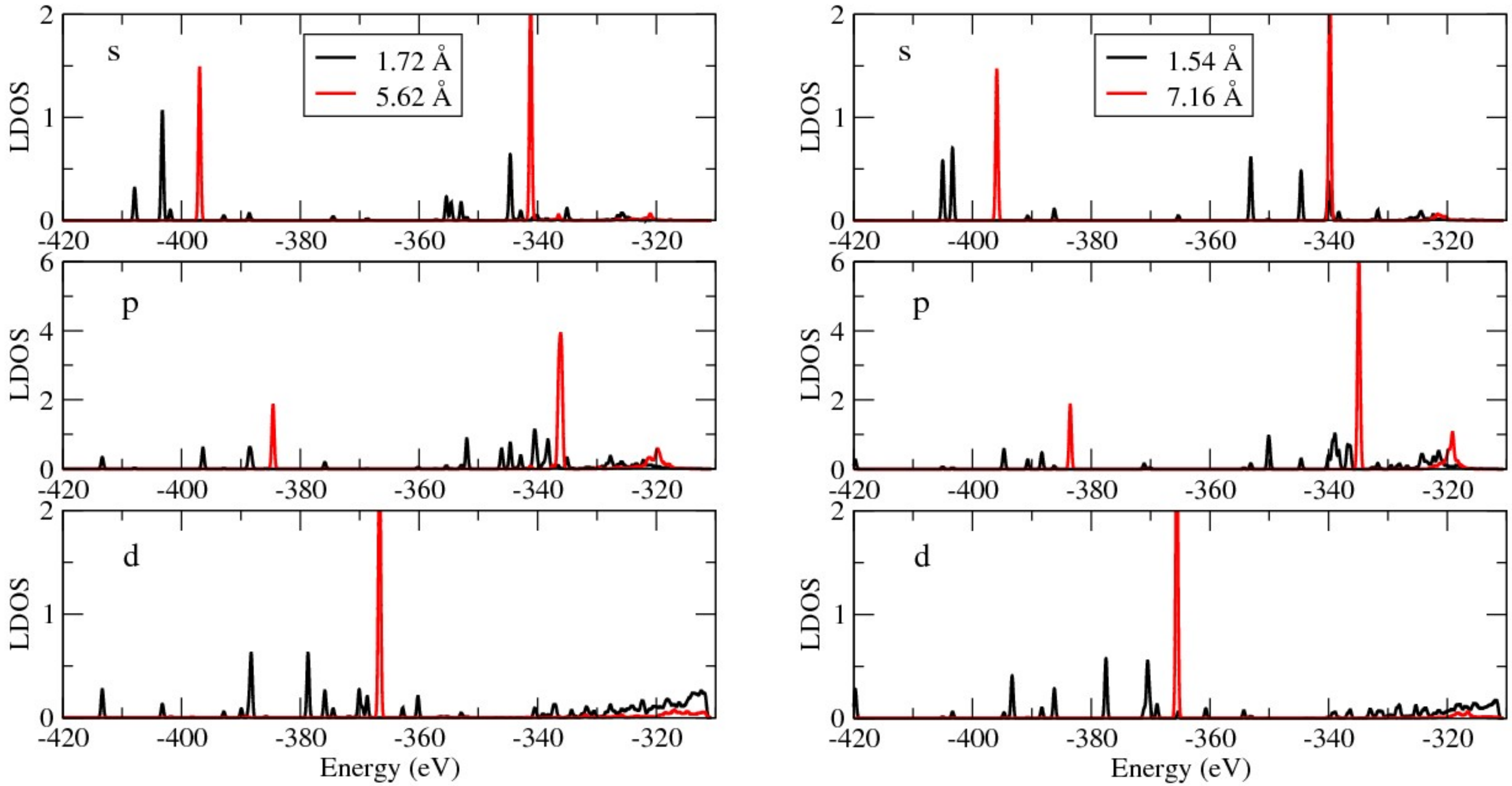




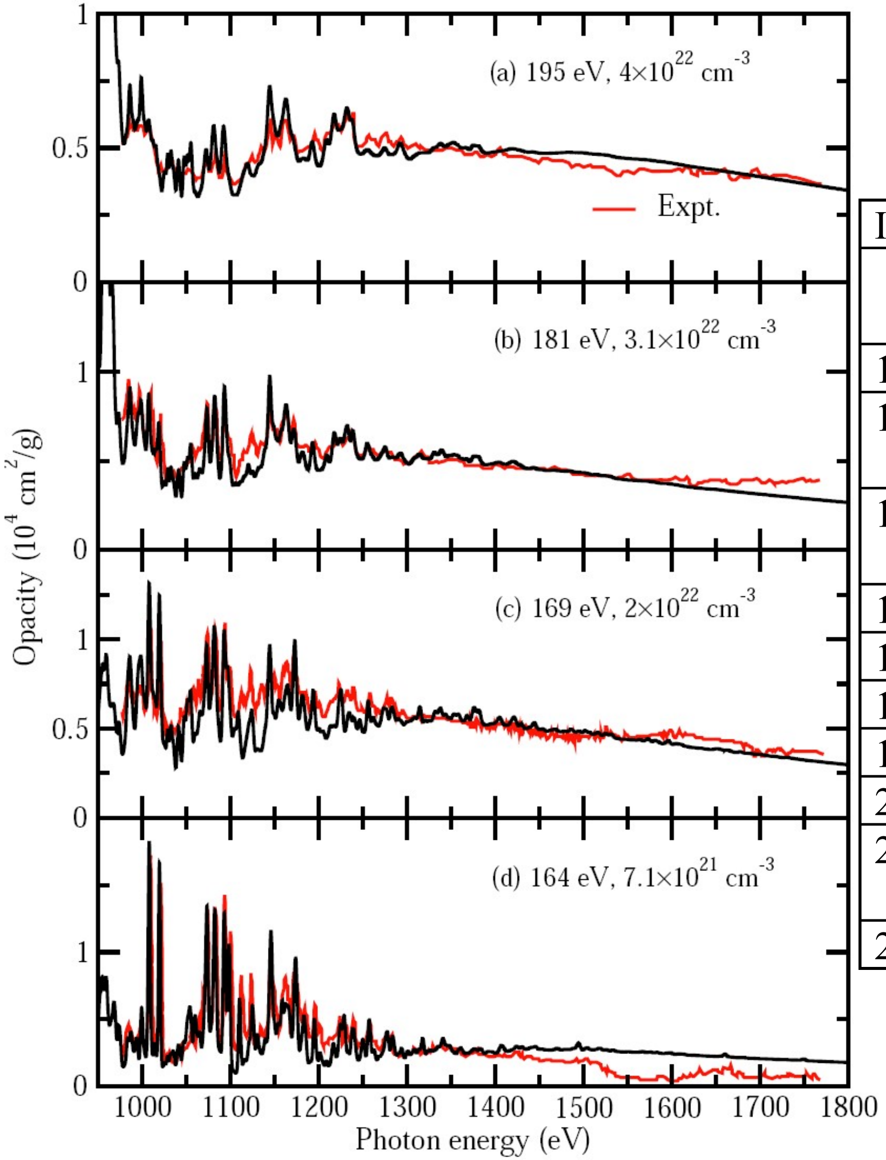
DFT based calculations with 16 atoms in a unit cell

Nuclear thermal motion driven electronic states

Two typical atoms chosen in the cell, one is close to another and one is separated from others.



Comparison with experiment using diagnosed CSDs



CSDs by Saha equation and diagnostics

Ion	195eV		181eV		169eV		164eV	
	Diag nose	Saha Eq.	Diag nose	Saha Eq.	Diag nose	Saha Eq.	Diag nose	Saha Eq.
13	0	0	0.02	0.0	0.05	0.0	0.0	0.0
14	0.01	0	0.07	0.003	0.05	0.004	0.0	0.0
15	0.01	0.012	0.10	0.22	0.20	0.03	0.0	0.005
16	0.14	0.11	0.15	0.16	0.18	0.18	0.28	0.07
17	0.32	0.30	0.25	0.36	0.24	0.39	0.30	0.27
18	0.28	0.35	0.23	0.32	0.17	0.30	0.18	0.40
19	0.18	0.18	0.12	0.12	0.02	0.09	0.01	0.22
20	0.01	0.04	0.01	0.02	0.01	0.01	0.04	0.04
21	0.05	0.0	0.05	0.001	0.08	0.0	0.03	0.003
22	0.0	0.0	0.0	0.0	0.00	0.0	0.16	0.0

Electron impact ionization processes

The energy differential cross section for the electron-impact ionization reads

$$\frac{d\sigma_{if}(\epsilon_0,\epsilon)}{d\epsilon} = \rho(\epsilon_0)\rho(\epsilon)\rho(\epsilon_0 - I - \epsilon)\frac{2\pi}{k_i^2 g_i}\sum_{\kappa_i\kappa_f}\sum_{J_T}(2J_T+1)$$
$$|\langle\psi_i\kappa_i, J_T M_T|\sum_{p<q}\frac{1}{r_{pq}}|\psi_f\kappa_1\kappa_2, J_T M_T\rangle|^2, \tag{3}$$

where $\rho(\epsilon)$ is the density of states of the corresponding continuum electron [15], I the ionization potential, g_i the statistical weight of the initial state, k_i the kinetic momentum of the incident electron, J_T the total angular momentum when the target state is coupled to the

Electron impact ionization processes

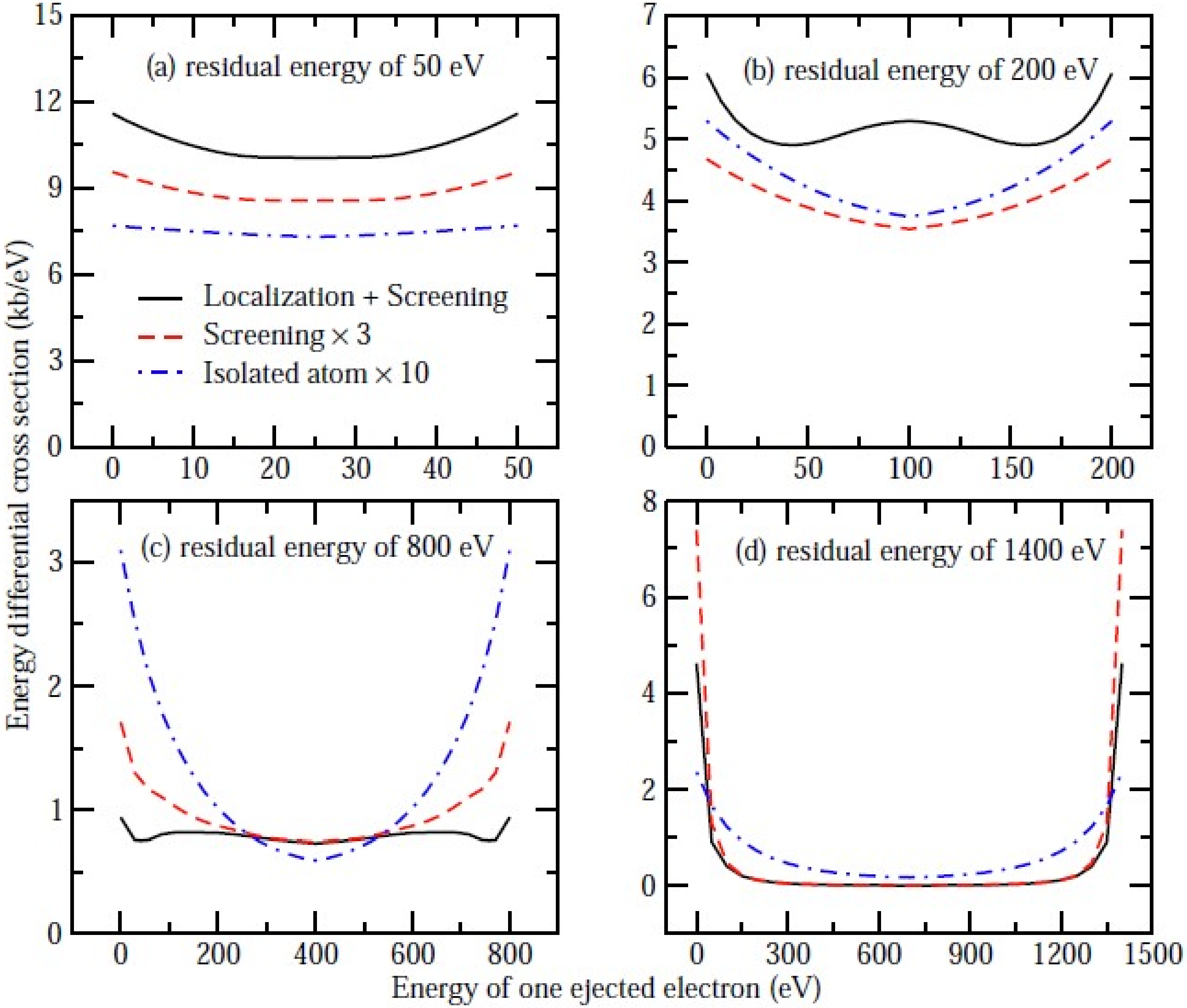


FIG. 1. Energy differential cross section of electron–ion collisional ionization of Mg^{9+} $e+1s^22s\ ^2S \rightarrow 1s^2\ ^1S+2e$ occurring in a solid-density magnesium plasma at a temperature of 150 eV with a residual energy of (a) 50 eV, (b) 200 eV, (c) 800 eV, and (d) 1400 eV. For clarity, the results obtained with the isolated-ion and screened-ion models are multiplied 10- and 3-fold, respectively.

Electron impact ionization processes

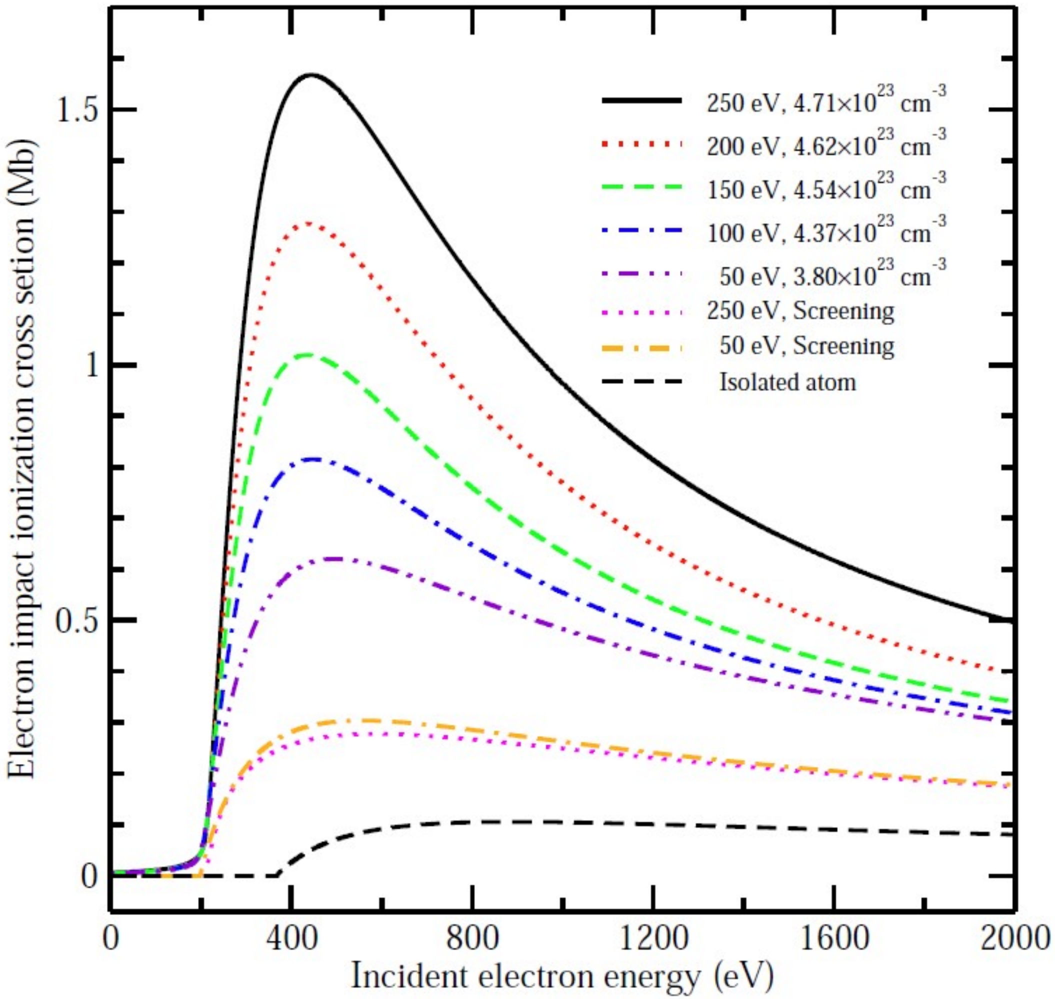


FIG. 2. Enhanced integrated cross section in electron–impact ionization of Mg^{9+} $e+1s^22s\ ^2S \rightarrow 1s^2\ ^1S+2e$ occurring in solid-density magnesium plasma at temperatures of 250 eV, 200 eV, 150 eV, 100 eV, and 50 eV. The integrated cross sections obtained by the screened ion model are weakly temperature dependent and hence for clarity only the results at the highest (250 eV) and lowest (50 eV) temperatures are given.

Electron impact ionization processes

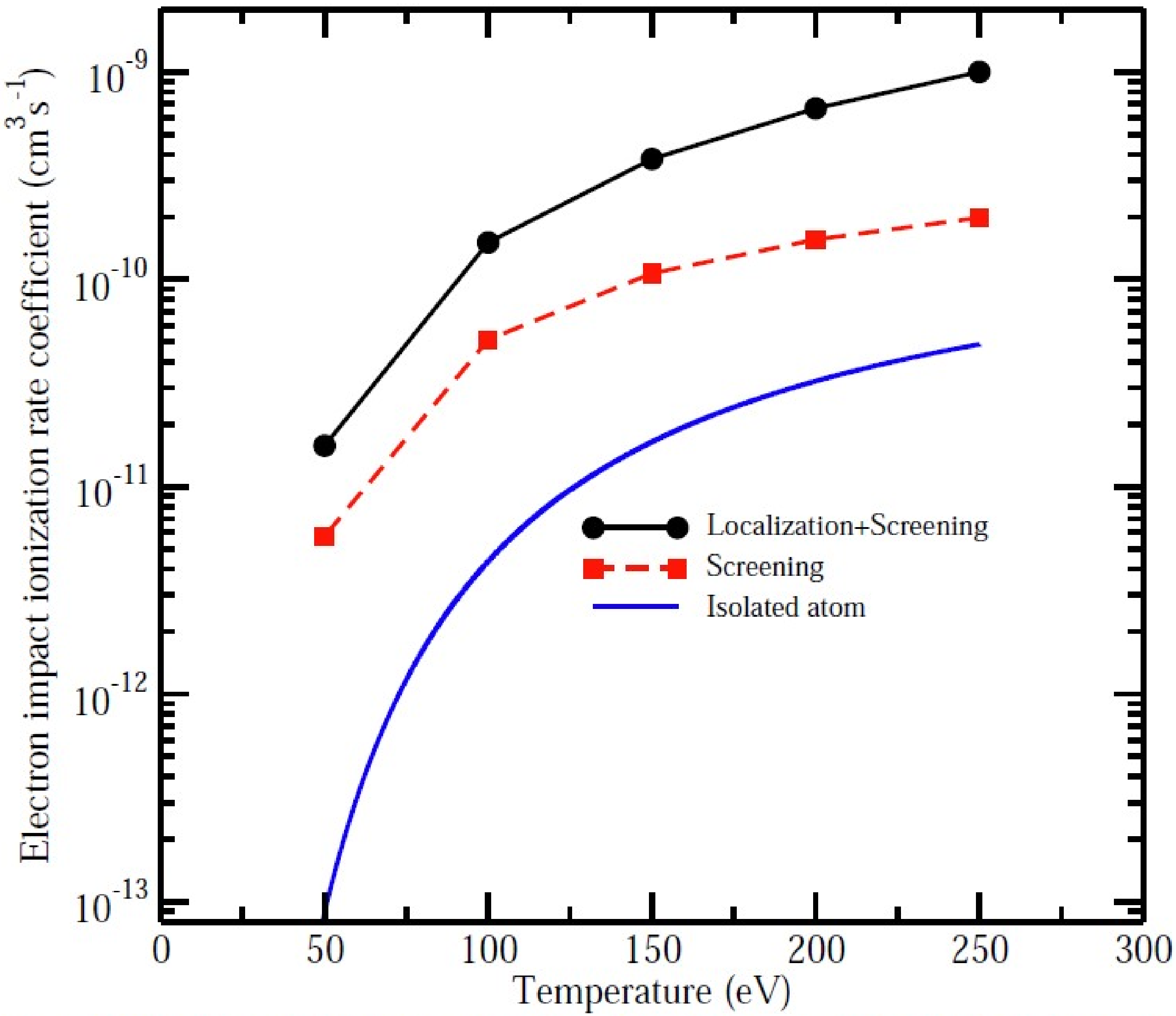


FIG. 4. Electron-ion collisional ionization rates as a function of plasma temperature for the solid-density magnesium plasma.

Electron impact ionization processes

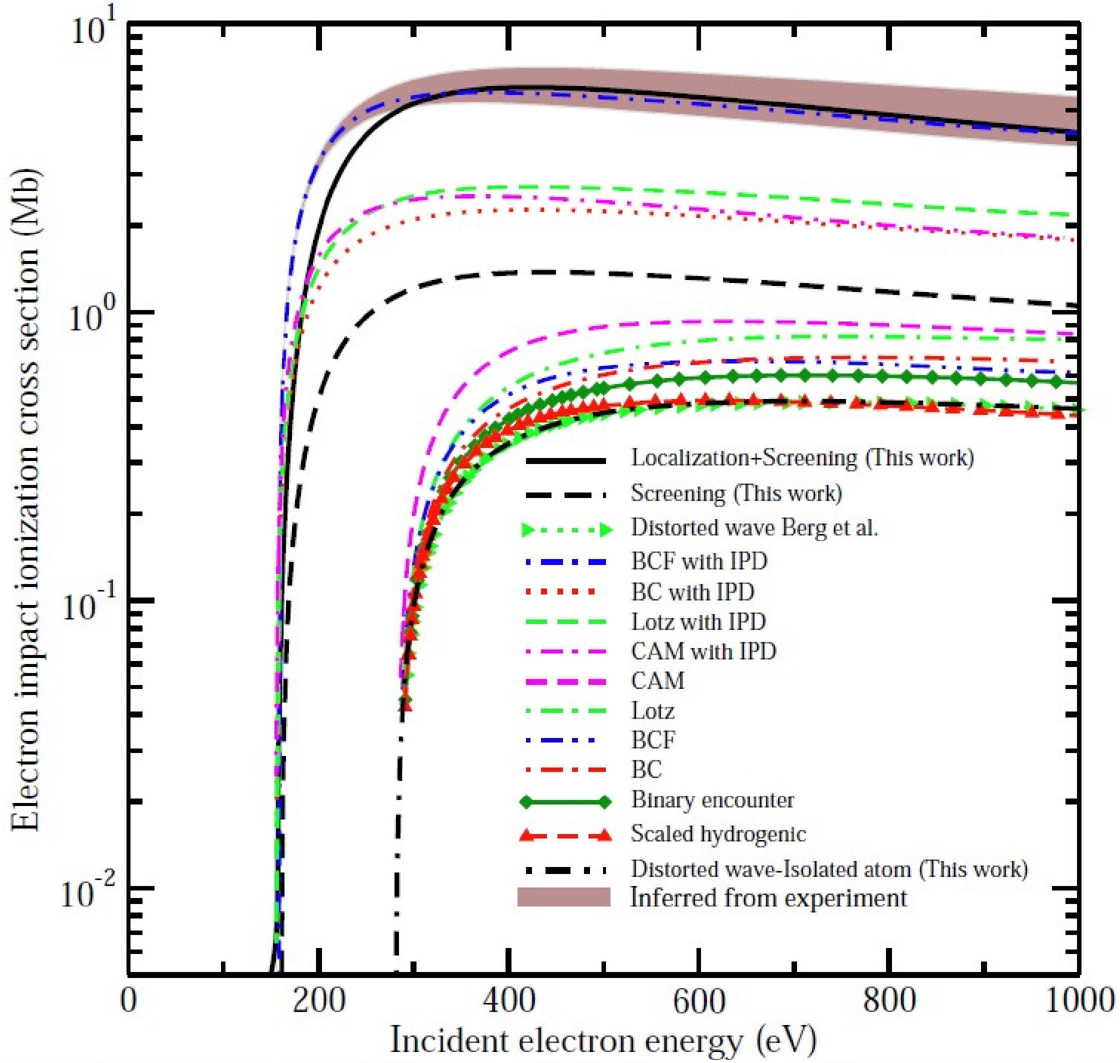


FIG. 5. Collisional ionization cross section of Mg^{7+} $e+1s2s^22p^2\ ^2P_{1/2} \rightarrow 1s2s^22p+2e$ occurring in solid-density magnesium plasma at a temperature of 75 eV. The cross sections we obtained are compared with the result inferred from the experiment by Berg and colleagues [14], and theoretical calculations using different methods of Lotz [29] and the revision by Burgess and Chidichimo (BC) [30], the scaled hydrogenic approximation [31] and its analytic fitting formula by Clark, Abdallah, and Mann (CAM) [32], binary encounters [33], and the distorted wave approximation [34] and the BCF with and without IPD model.

Summary

1. Here we propose the notion of a transient space localization of electrons produced during the ionization of atoms immersed in a hot dense plasma.
2. A theoretical formalism is developed to study the wavefunctions of the continuum electrons that takes into consideration the quantum de-coherence caused by coupling with the plasma environment.
3. We find that the cross section is considerably enhanced compared with the predictions of the existing isolated-atom model.
4. And thereby partly explains the big difference between the measured opacity of Fe plasma and the existing standard models for short wavelengths, and also explains the big gap between the extracted electron impact ionization rates from laser heated Mg plasma and the calculated values using the existing models.

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Thanks for your attention!