Study of the statistical and radiative properties of dense plasma.

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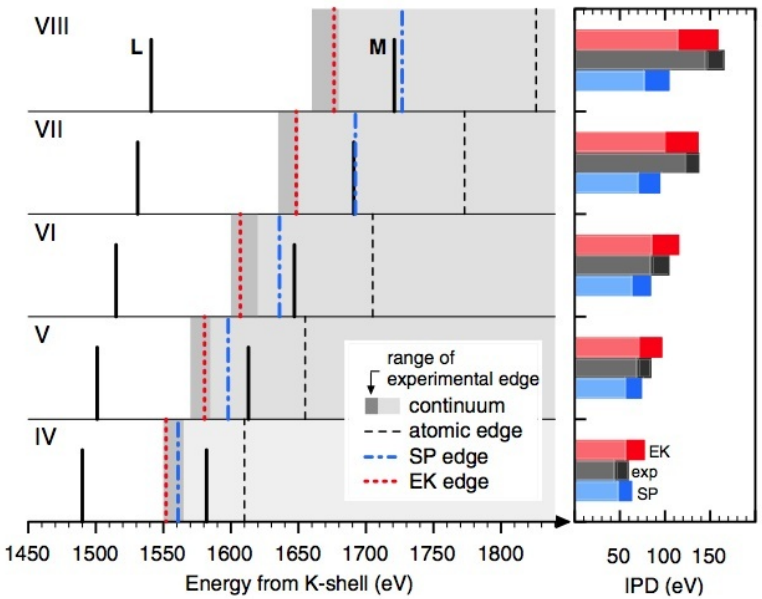
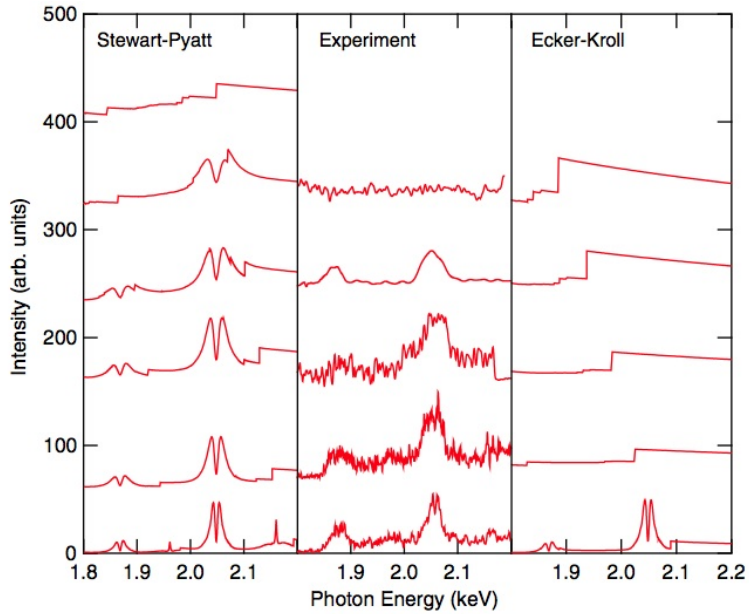
Introduction

The radiative properties of an atom or an ion surrounded by a plasma are modified through various mechanisms.
Depending on plasma conditions, the electrons supposedly occupying the upper quantum levels of radiators no longer exist.
All the charges of the plasma contribute to the lowering of the energy required to free a bound electron.
This mechanism is known as ionization potential depression (IPD).
The evaluation of the IPD has important implications for dense plasma physics and in particular for the detailed prediction of the dense plasma equation of state and radiative opacity in stellar interiors, inertial confinement fusion research, or planetary interiors.

Introduction

Experiments performed a few years ago [1, 2] leading to IPD measurements in situ renewed interest for this issue.
There are several theoretical IPD models that apply to various conditions. Two of them, the Stewart-Pyatt (SP) [3] and the Ecker-Kröll (EK) [4] model, which apply across a wide range of densities, allow a general discussion of these experiments.

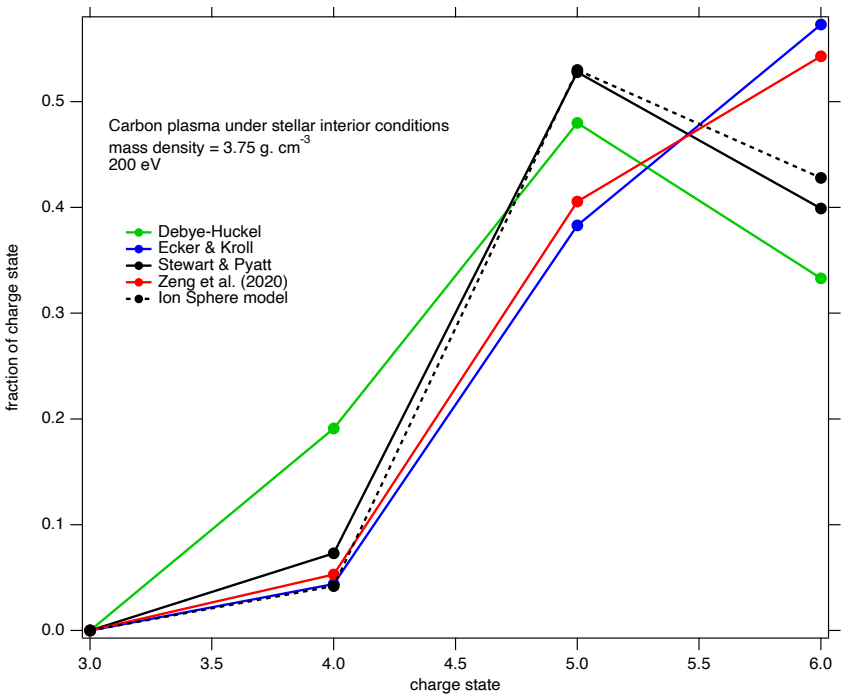


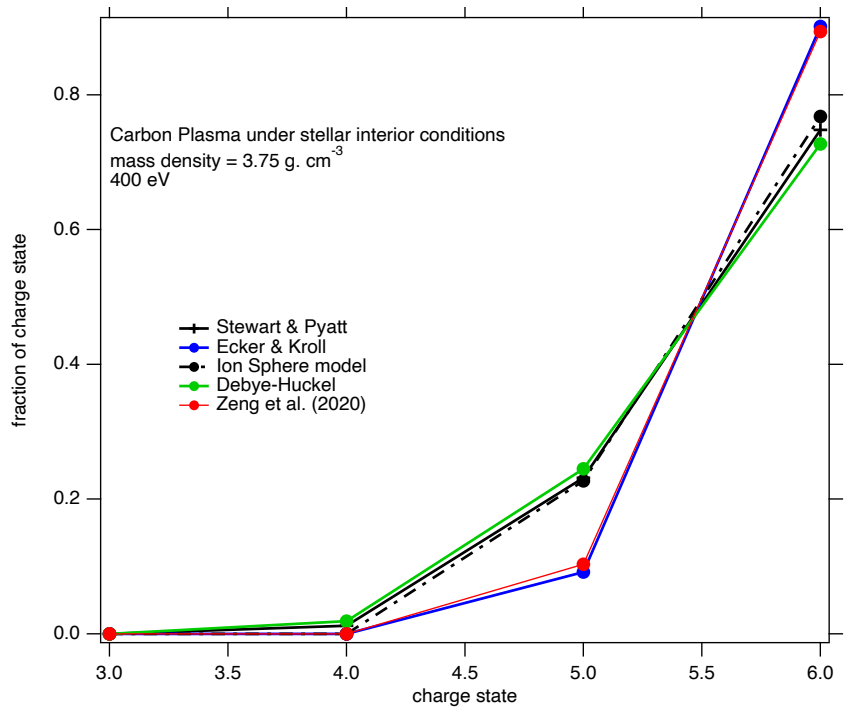


[1] O. Ciricosta et al., PRL 109 (2012) 065002 ; O. Ciricosta et al., Nat. Commun. 7 :11713 (2016).
[2] D.J. Hoarty et al., PRL 110 (2013) 265003.
[3] J. Stewart and K. Pyatt, Jr., Astrophys. J. 144, 1203 (1966).
[4] G. Ecker and W. Kröll, Phys. Fluids 6, 62 (1963).

Introduction

An accurate description of IPD plays an essential role in determining the charge state distribution and ionization balance. Hereafter the results obtained by Zeng et al. [5] for Carbon plasma in stellar interior conditions :





[5] Zeng J. et al., A&A 644, A92 (2020).

Introduction

The evaluation of the IPD requires dealing with highly complex n-body coupled systems, involving particles with different dynamics and attractive ion-electron forces.

A plasma contains at least two components (electrons and ions) and most systems have more than one ion species. In strongly coupled plasmas, the behavior of ions and electrons is intrinsically linked to the surrounding plasmas. Electromagnetic interactions between charged particles induce collective behavior of ions and electrons. When the potential energy becomes larger than the thermal energy, particles are strongly correlated, affecting the structural and dynamical properties of the medium.

Introduction

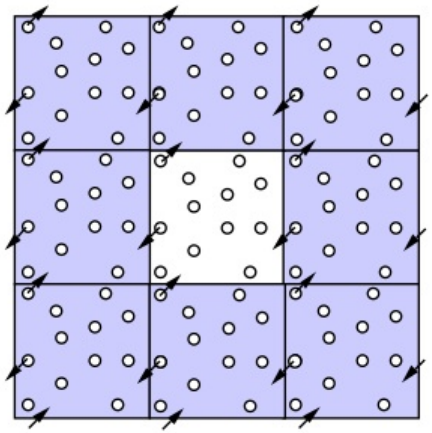
A classical multi-component plasma molecular dynamics (MD) code, the BINGO-TCP code, has been developed to follow the evolution of plasmas involving ions of various charge states [6].

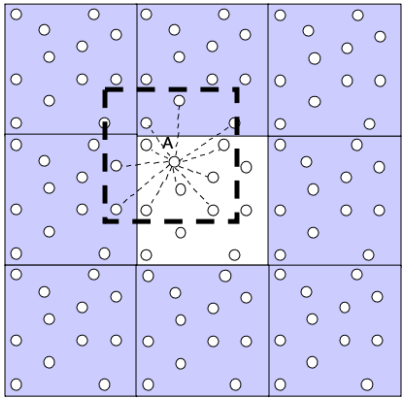
- Find a soft ion-electron potential which removes Coulomb divergence at short distances and accounts for some quantum effects.
- Implement a ionization/recombination protocol to control the plasma ion charge distribution and the trapping of electrons in the ion wells.

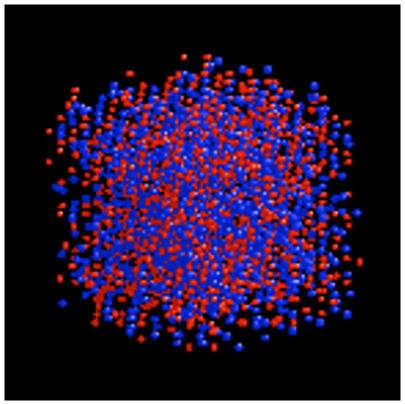
Within the limits of classical mechanics, all charge-charge interactions are accounted for in the particle motion.

[6] A. Calisti, S. Ferri and B. Talin, J. Phys. B : At. Mol. Opt. Phys. 48, 224003 (2015).

The BinGo-TCP code







Simulation of the movement of classical non relativistic point-like interacting particles.
In a three dimensional infinite system in thermodynamical equilibrium composed of joint identical cubic cells.
All the step by step calculation work done into a unique cubic cell with the so called minimum image convention.
Periodic boundary conditions are used and the Newton's equations are solved using a Velocity-Verlet algorithm.

Modeling

MD and soft potentials.

Simulating ions and electrons together can be performed provided that an ion-electron potential finite at short distances avoid electron-ion collapse. Such effective regularized potentials are designed to approximately account for known quantum properties appropriate for the kind of investigated plasma :

- quantum interference and diffraction effects at small distances involved in electron-electron or electron-ion collisions for hydrogenic systems [7]
- the correct ionization energy of the ions in the ground state when the electrons are situated on top of the ions for nano plasma properties. [8]

We have chosen to simulate the ions and electrons as classical particles and to incorporate a minimum of quantum information through a regularized potential allowing to modelize collisional ionization and recombination processes.

[7] H. Minoo, M. M. Gombert, and C. Deutsch, Phys. Rev. A 23, 924 (1981).

[8] M. Belkacem, et al., Eur. Phys. J. D 40, 247255 (2006).

Modeling

MD and soft potentials.

The system inside the simulation box is neutral.
Electron-electron or ion-ion interactions are taken to be Coulomb :

$$V_{ii,ee} = Z_{i,e}^2 e^2 e^{-r/\lambda}/r.$$

The interactions are screened at a distance $\lambda \simeq s/2$.
For opposite charges, a regularized potential at short and large distances is used :

$$V_{ie}(r) = -Z_i e^2 e^{-r/\lambda}(1 - e^{-r/\delta(Z_i)})/r.$$

The regularization distance δ is associated to the ionization energy of each ion stage :

$$\delta(Z) = -Ze^2/E(Z).$$

An electron located at an ion ($r = 0$) occupies the fundamental state of the ion whose charge is Z with a nucleus charge $Z + 1$.

Modeling

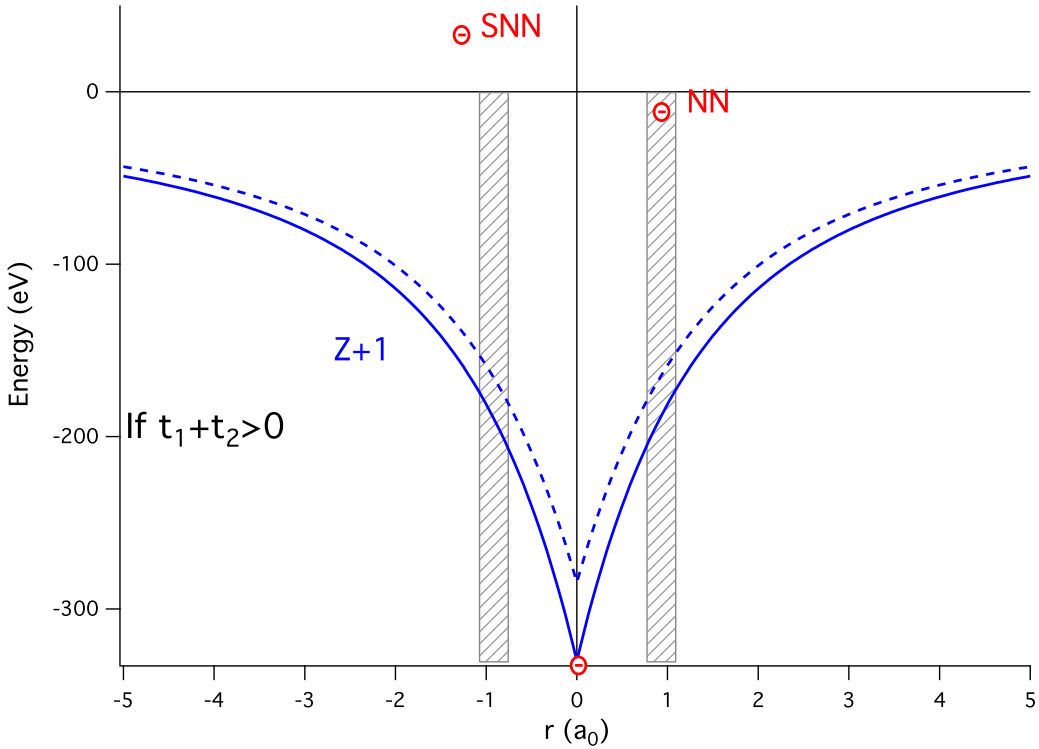
Specific difficulties.

- We use very small timesteps $\approx 10^{-20}$s appropriate for the description of the micro motion of electron around ions.
- Time steps are small compared to typical collision rates $\Rightarrow$ **statistics on collisional events are expensive.**
- The setting up of the population of electrons temporary trapped in the ion wells depends on collisional events between electrons, and thus, is **a very slow process**.
- The choice of the ion-electron potential associated to the knowledge of the position and velocity of individual particles at each time step, allows us to design a collisional ionization-recombination process.
- Ionization-recombination mechanisms rely on an approximate analysis of collisional events between one ion and 1 or 2 electrons. The concept of collisions is not straightforward as the interaction involves all particles within the screening length.
  $\Rightarrow$ **The definition of a collisional process is crucial but necessarily empirical.**

Modeling

Ionization-recombination model.

The location of the two nearest neighbor electrons and the sign of their total energy is used to evaluate if locally the plasma, at one step of its evolution, is favorable to an ionization (positive energy) or a recombination (negative energy) of the ion.

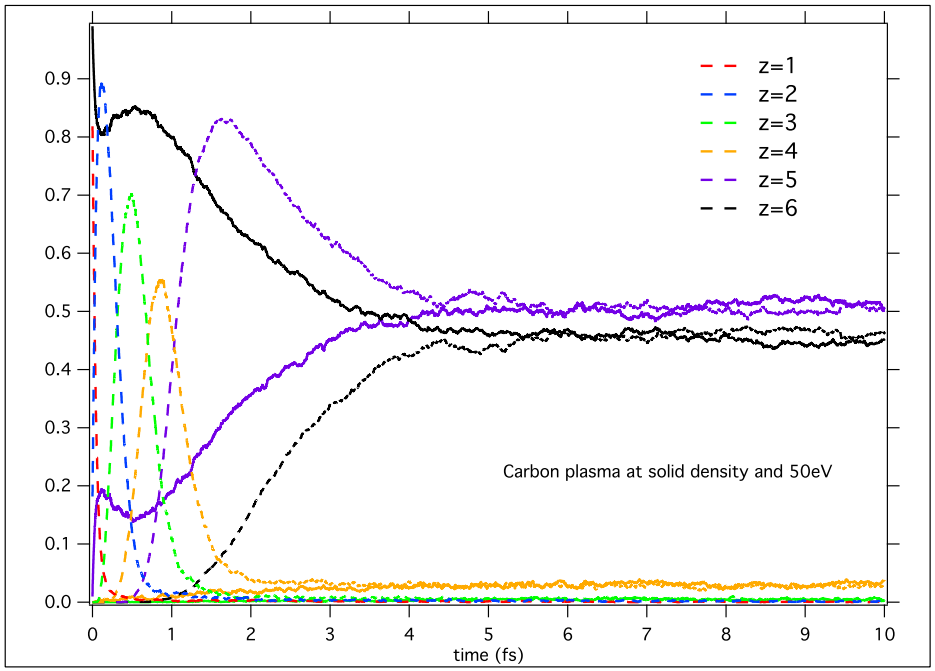


Modeling

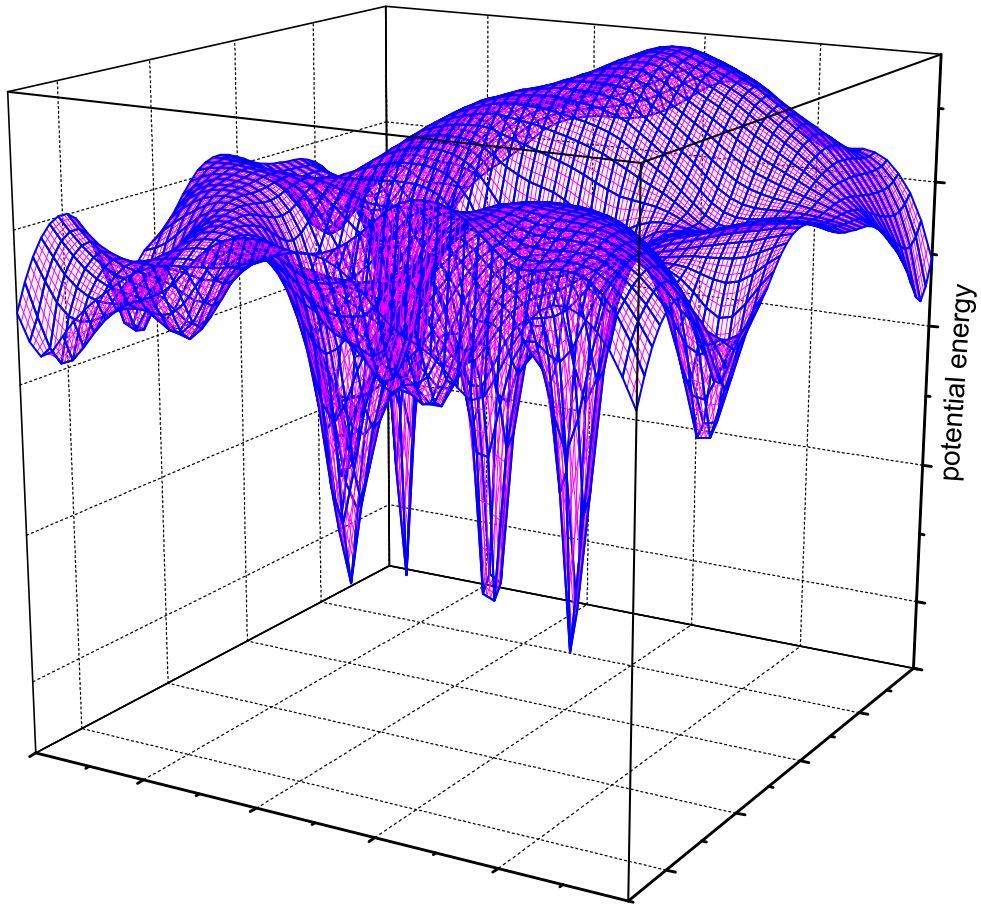
This ionization/recombination process implemented in the code has two fundamental functions :

- It allows the evolution of the charge state population towards a stationary state depending on temperature, density and composition of the plasma.
- It favors the setting up of a population of electrons temporary trapped in the ion wells.

A preparation phase of the particle set (into the simulation box) before extracting any sampling from simulations, is necessary. At the end of the preparation phase the system follows a quasi stable evolution with stationary trapped and free electron populations.



Modeling



Applications.

Ionization potential depression.

The ionization potential of an ion imbedded in a plasma is lowered due to the whole charged particles (ions and electrons) interacting with that ion.

The study of IPD is illustrated and discussed for aluminum and magnesium plasmas in the conditions of the experiments [1] and [2] mentioned in the introduction, and also for dense Carbon plasma under solar interior conditions.

[1] O. Ciricosta et al., PRL 109 (2012) 065002 ; O. Ciricosta et al., Nat. Commun. 7 :11713 (2016).
[2] D.J. Hoarty et al., PRL 110 (2013) 265003.

Ionization potential depression

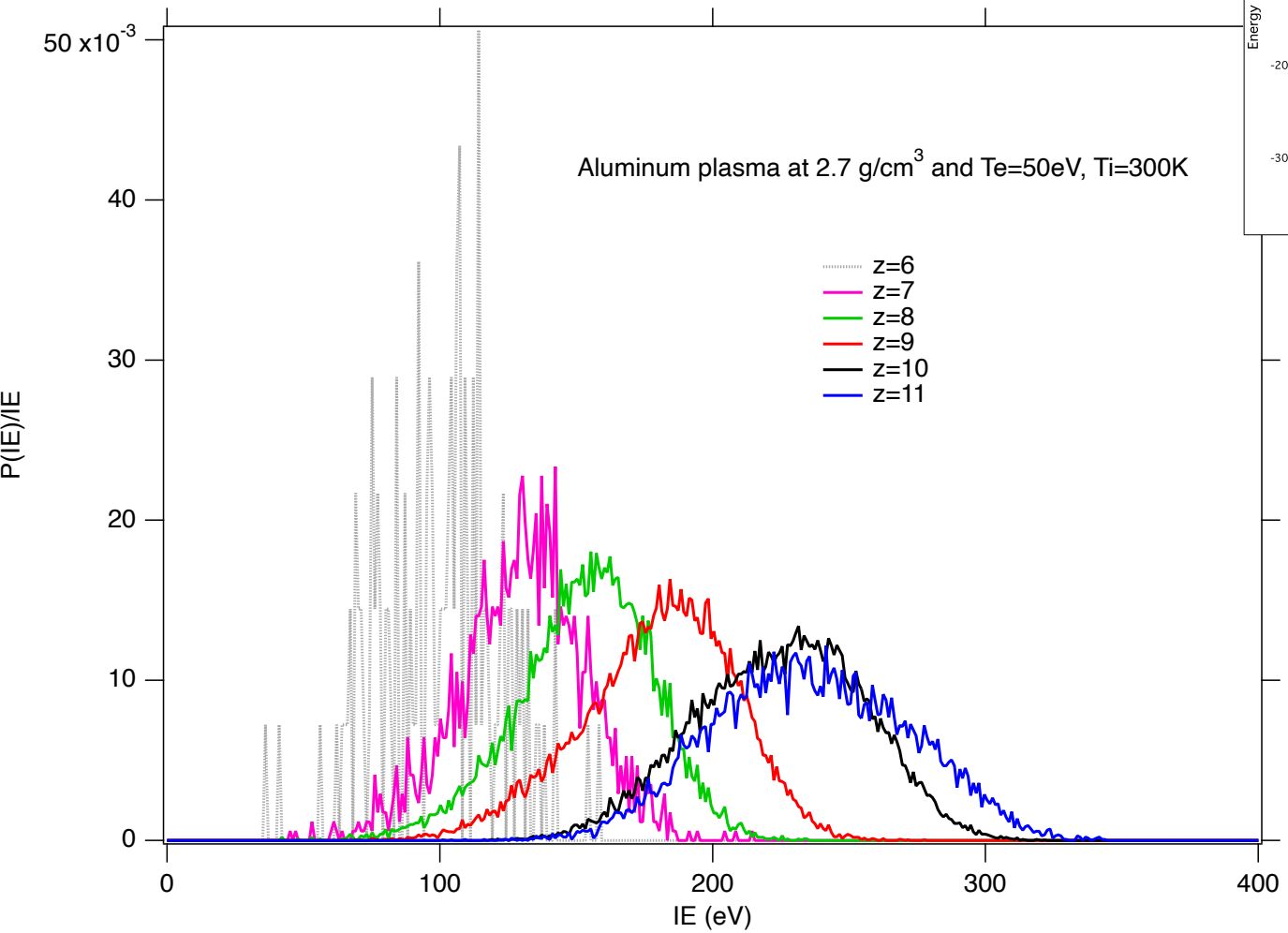
Experimental conditions

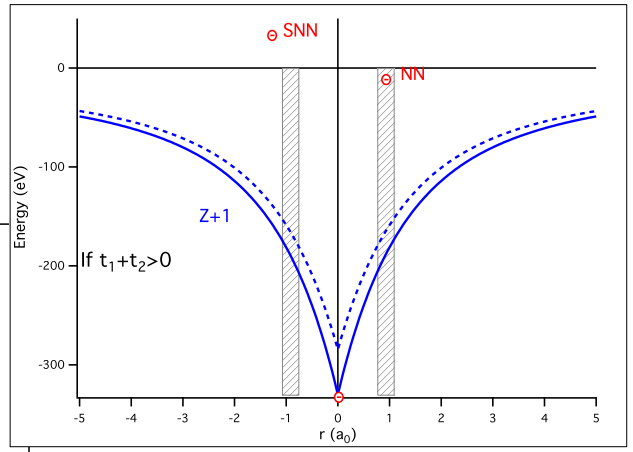
The BinGo-TCP code has been used to match approximately the conditions of O. Ciricosta experiment, with typically the ion temperature, $T_i = 300$K and the electron temperature, $T_e = 50$eV.
The argument here is that the electron adjustment to the ions can occur in a time that does not allow the ion population to be heated by the electrons.

For the IPD measurement, the method relies on a sampling of the total potential energy of the electron located at an ion being ionized. The potential energy of such an electron results from the whole interacting charged particles interacting with it.

Ionization potential depression.

Aluminum, $\rho = 2.7$ g.cm^{-3}





Ionization potential depression.

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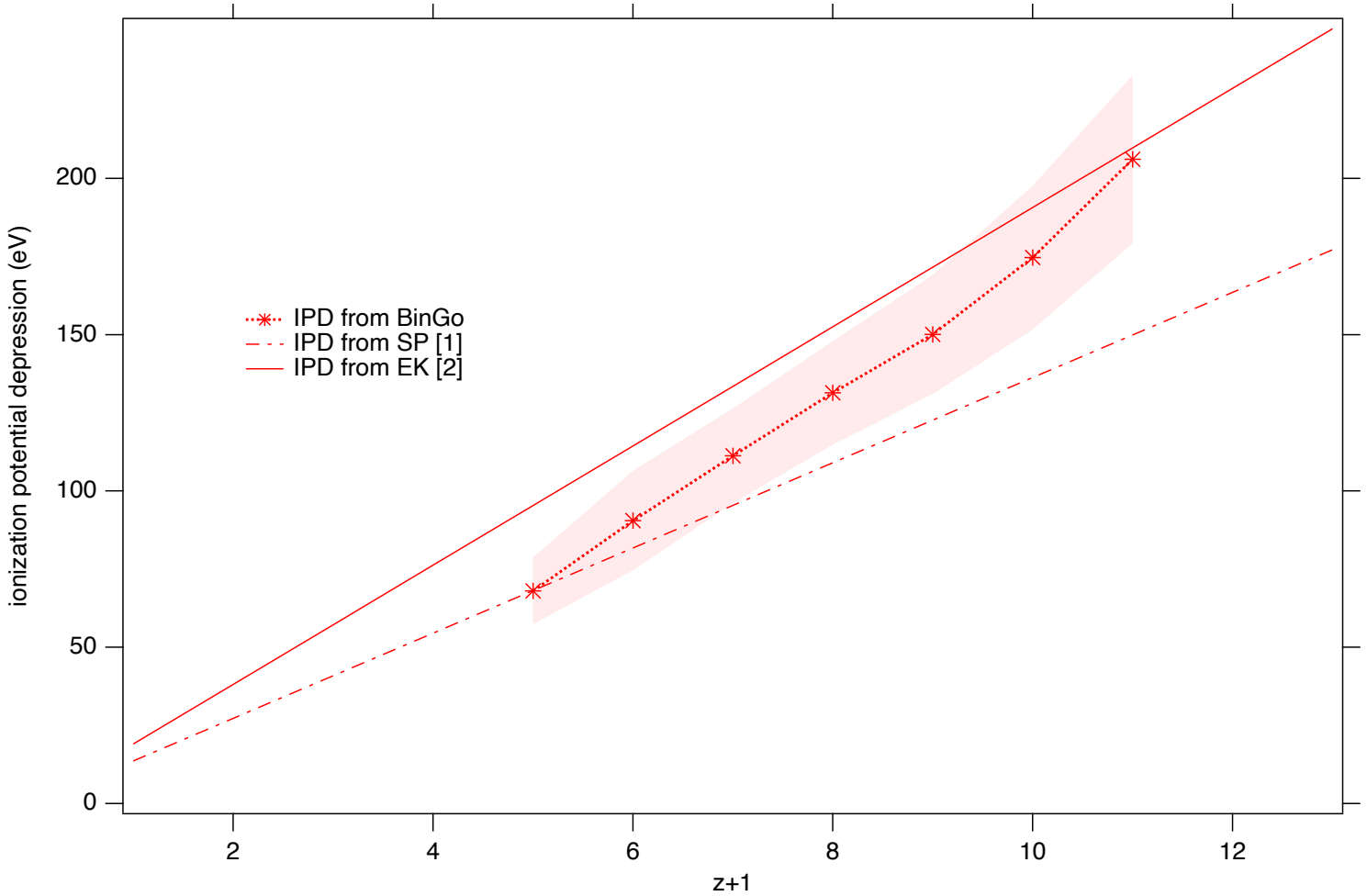

J. Stewart and K. Pyatt, Jr., Astrophys. J. 144, 1203 (1966).
G. Ecker and W. Kröll, Phys. Fluids 6, 62 (1963).

Ionization potential depression.

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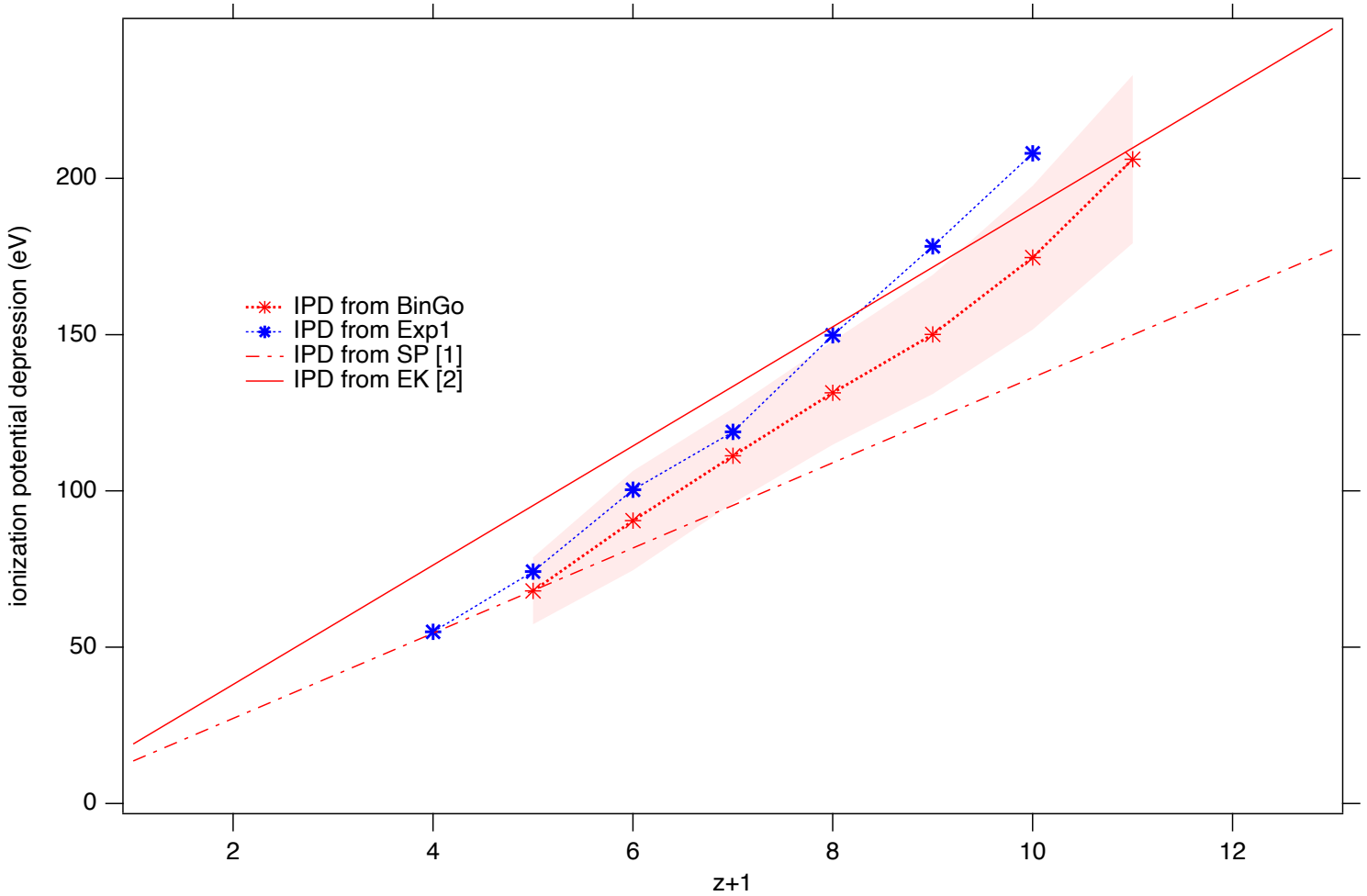
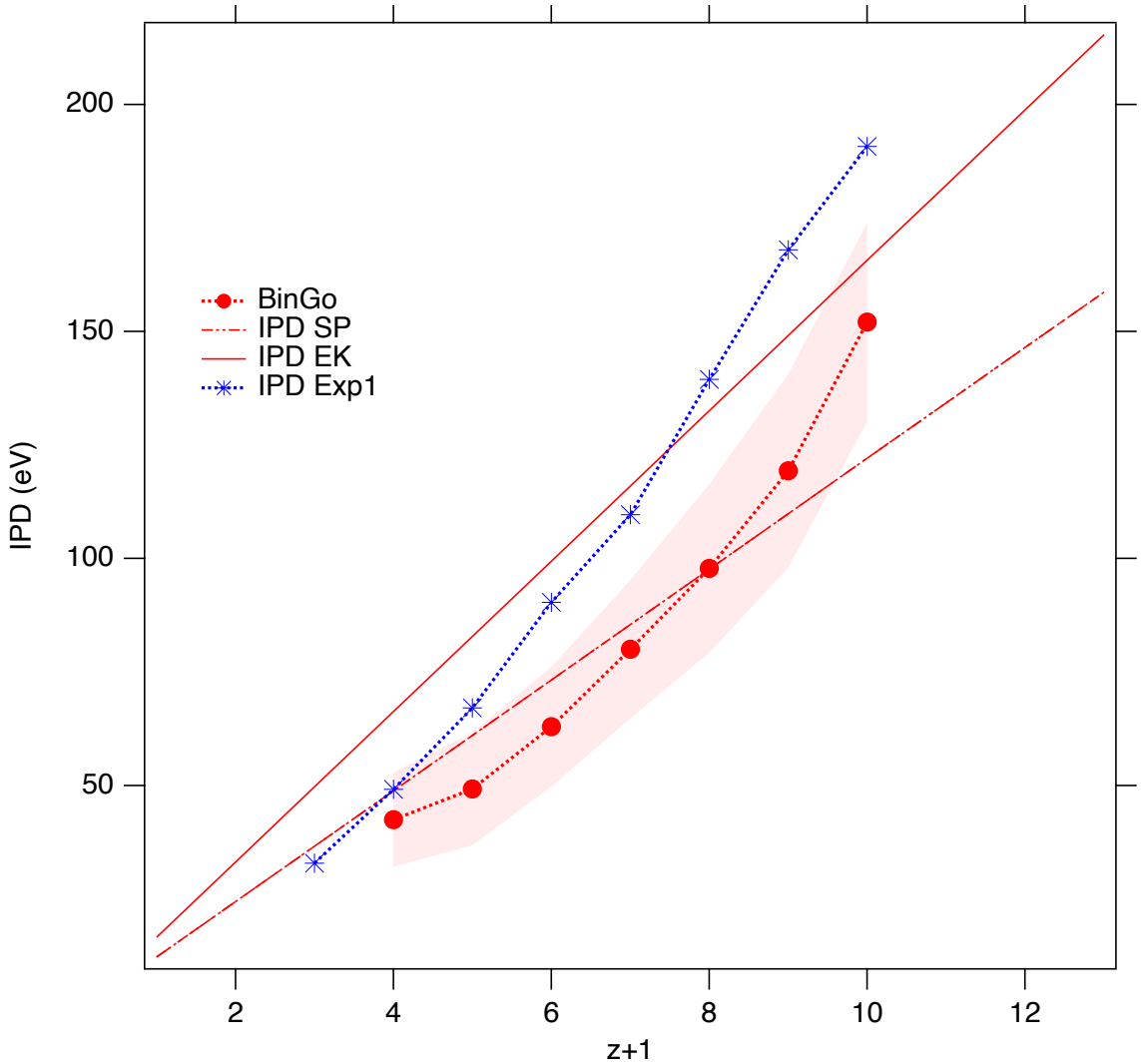
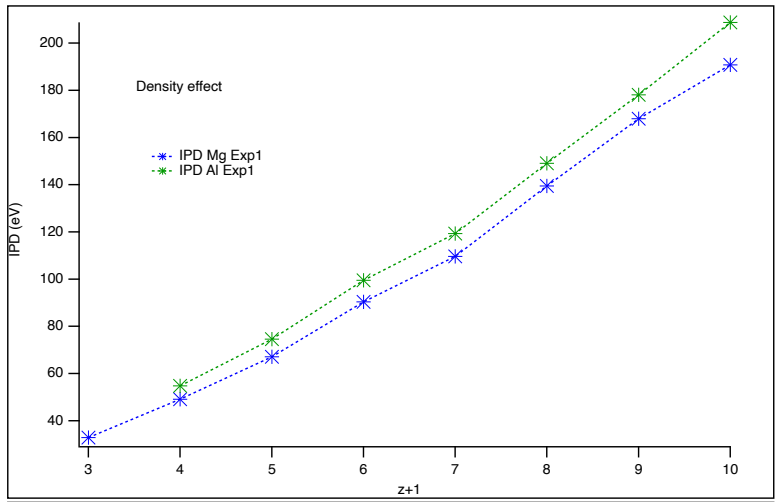


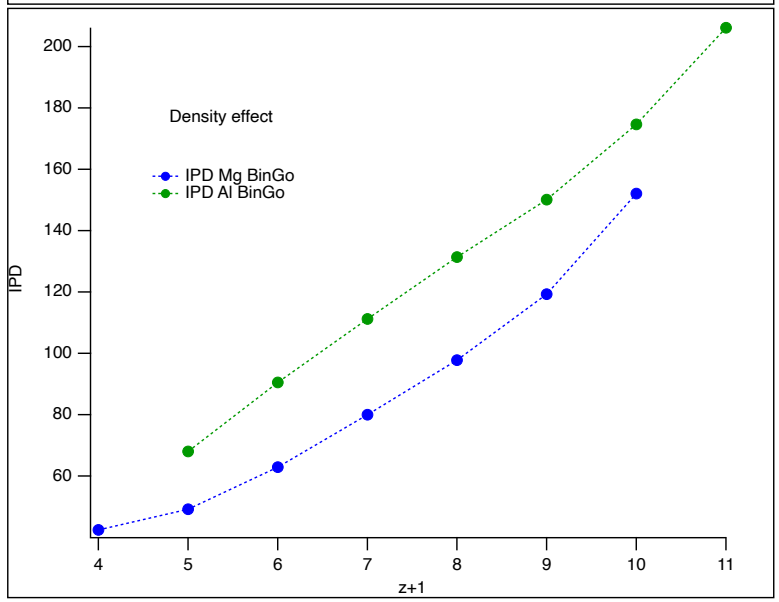
J. Stewart and K. Pyatt, Jr., Astrophys. J. 144, 1203 (1966).
G. Ecker and W. Kröll, Phys. Fluids 6, 62 (1963).
[*] O. Ciricosta et al., Nat. Commun. 7 :11713 (2016).

Ionization potential depression.

Magnesium, $\rho = 1.74$ g.cm^{-3}



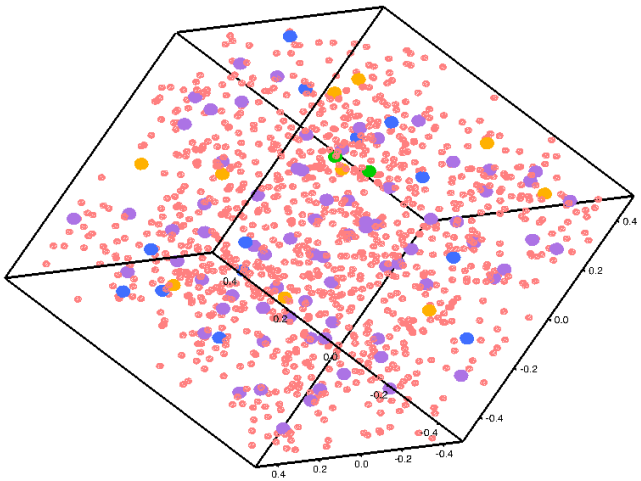


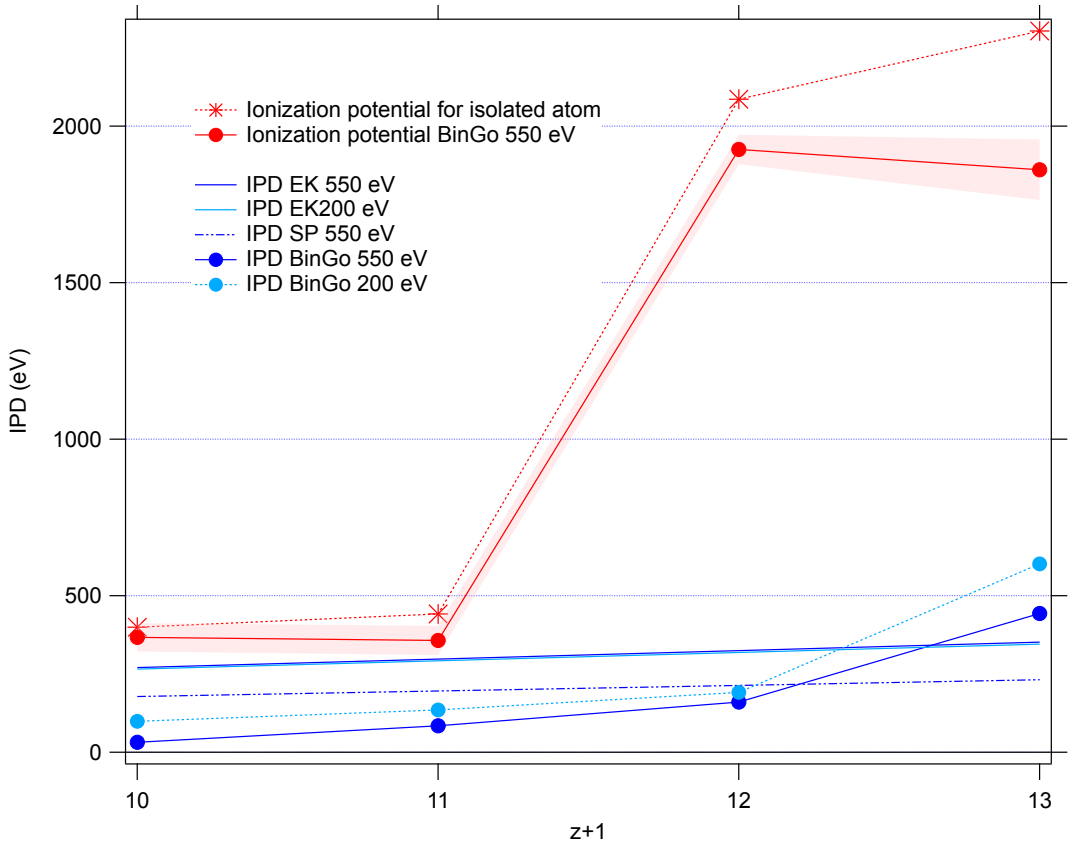


Ionization potential depression.

Aluminum, $\rho = 6.0$ g.cm^{-3}

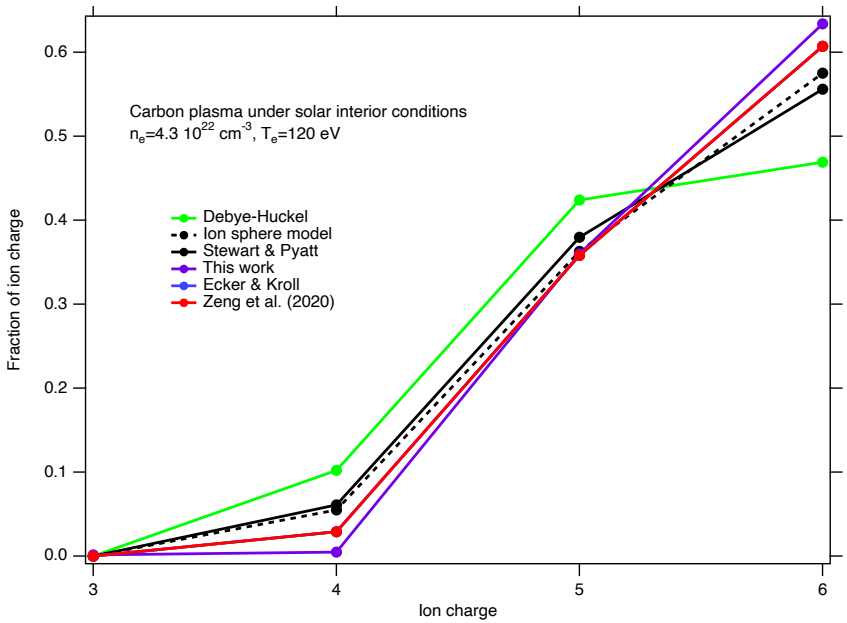
Here, $Te = Ti = 550eV$ in the conditions of Exp2 and $Te = Ti = 200eV$ for temperature effect.

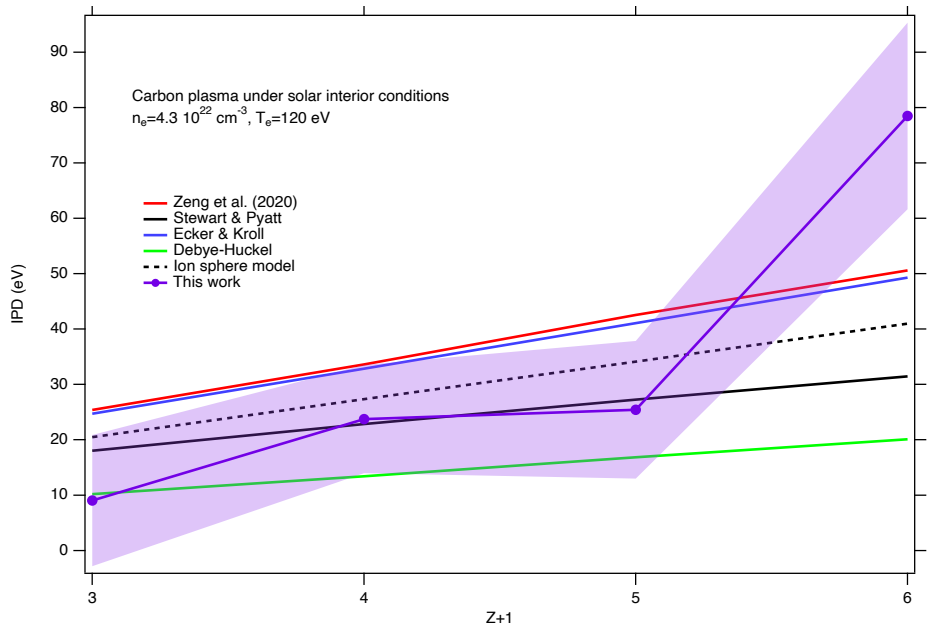




Ionization potential depression.

Carbon plasma under solar interior conditions



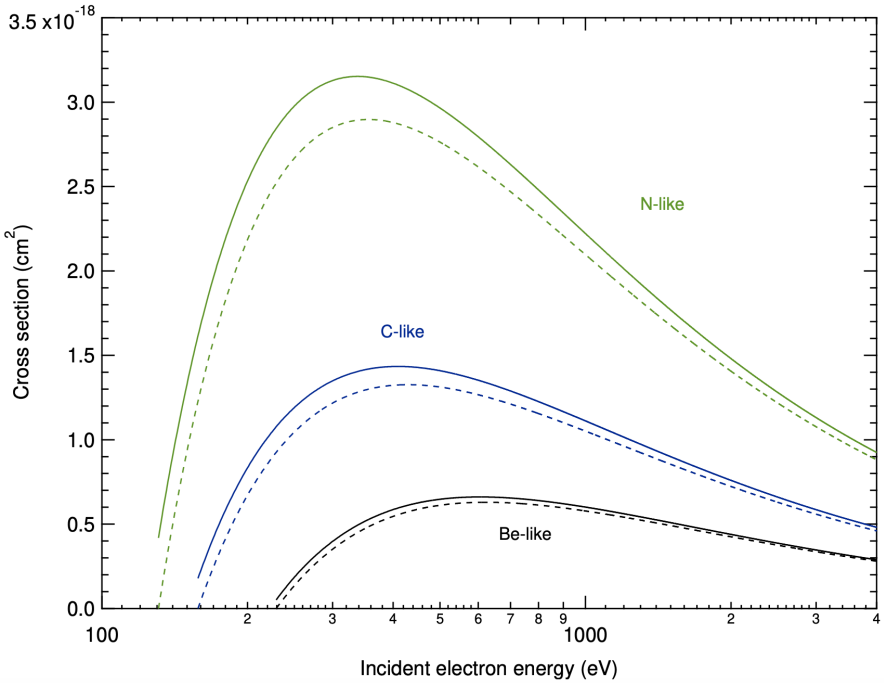


$n_e = 4.3 \times 10^{22} cm^{-3}$, $T_e = 120$ eV.

Plasma conditions deduced from the standard solar model at radius fraction of $0.796 R_\odot$

Cross-section of ionization by free-electron impacts.

Our Molecular Dynamics approach provides distributions of the ionization energy. These distributions result from the fluctuations of the ionic charge environment.
IPD models do not account for fluctuations. We present here the influence of these fluctuations on the cross-section calculated with the Lotz formula.



$$\sigma(E|E_{i,av}) = A\xi \frac{ln(E/E_{i,av})}{EE_{i,av}}$$

$$\sigma(E) = <\sigma(E|E_i)>_P = A\xi \int \frac{ln(E/E_i)}{EE_i} P(E_i) dE_i$$

W. Lotz, J. Opt. Soc. Am. 57, 873 (1967).
D. Benredjem, J.C. Pain, A. Calisti, S. Ferri, submitted to PRE.

Conclusion

Our aim in developing the BinGo-TCP code was to avoid excess of complexity of models in order to preserve a straightforward interpretation of physics from simulation results.
The results obtained with our TCP-MD simulation code are very encouraging. They compare well with results obtained by other models or simulations and experimental results when they exist.
Our simulations provide data for further discussion on IPD models and more generally on the charge correlation effects on the plasma properties.