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## Ion induced radiation damage on the molecular level

Alvarado Chacon, Fresia

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## Atomic units and conversion factors

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The atomic units (a.u.) originate from the typical dimensions of the hydrogen atom. The length is the classical Bohr radius  $a_0$  of the ground state electron, the velocity  $\alpha c$  is the classical velocity of the electron in the ground state of hydrogen, and the time is the ratio of the length and velocity. The charge in atomic units is the charge of the electron, the mass is the mass of the electron and the energy is the sum of the kinetic and the potential energy of the hydrogen 1s electron,  $2 \times 13.6$  eV. An overview of the most important quantities is given in the following table 1. The atomic unit system is based on the following definition:

$$\hbar = m_e = e = 4\pi\epsilon_0 = 1, \quad (1)$$

where  $\hbar$  is Planck's constant divided by  $2\pi$ ,  $m_e$  and  $-e$  are the mass and the charge of the electron, respectively, and  $\epsilon_0$  the permittivity of free space.

Throughout this thesis both the projectile velocity in a.u. and its kinetic energy in keV/amu are used. For non-relativistic collision energies the relation between them is given by:

$$v \text{ (a.u.)} = 0.20 \sqrt{E \text{ (keV/amu)}} \quad (2)$$

Some conversion factors of interest are given in table 2 in the backside of this page.

**Table 1:** *Atomic units*

length	$a_0$	$5.292 \times 10^{-11}$ m
time	$a_0/\alpha c$	$2.419 \times 10^{-17}$ s
velocity	$\alpha c$	$2.188 \times 10^6$ m/s
mass	$m_e$	$9.109 \times 10^{-31}$ kg
charge	$e$	$1.602 \times 10^{-19}$ C
energy	$m_e(\alpha c)^2$	$4.359 \times 10^{-18}$ J
angular momentum	$\hbar$	$1.054 \times 10^{-34}$ J s

**Table 2:** *Conversion factors*

1 amu	$1.660 \times 10^{-27}$	kg
	1822.888	$m_e$
1 a.u. energy	27.2116	eV
	627.5095	kcal/mol
1 cal	4.184	J