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Letter

Characterization of Rare Gas Atoms in Cold Dense Plasma

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By plotting the threshold energy as measured by Flynn and co-workers for Kr and Xe impurities in the alkali metals, it is demonstrated that the concept of an atom in a cold dense plasma is useful in the present context. The threshold energy of the rare gas is remarkably linear in the interelectronic spacing r_s between Li and Cs though it must saturate at the value of the first ionization potential for sufficiently large r_s .

Key Words: Excitation energy, plasma, virtual bound state.

The experiments of Flynn *et al.*¹ on rare gas impurities in the alkali metals have stimulated theoretical work on such atoms in jellium.² This idea of atoms in cold dense plasma³ is the focus of the present letter. It will be demonstrated that the threshold energy E_t , determined from the absorption measurements of Flynn *et al.*,¹ varies smoothly with interelectronic spacing r_s through the range of densities $3.2 < r_s < 5.5$ in Bohr radii a_0 , afforded by the alkali metal series Li to Cs. The way this threshold energy $E_t(r_s)$ can be characterized is then of obvious interest.

Figures 1 and 2 demonstrate the behaviour of E_t vs. r_s for Kr and Xe in the alkali metals. There is evidently a linear behaviour over the range from Li to Cs. The first ionization potentials I of the free atoms are to be noted: presumably at higher r_s curvature must occur so that $E_t \rightarrow I$ as $r_s \rightarrow \infty$. In each case for $r_s < \sim 5.5$, one may therefore write:

$$E_t = \varepsilon_0 + \varepsilon_1 r_s \quad (1)$$

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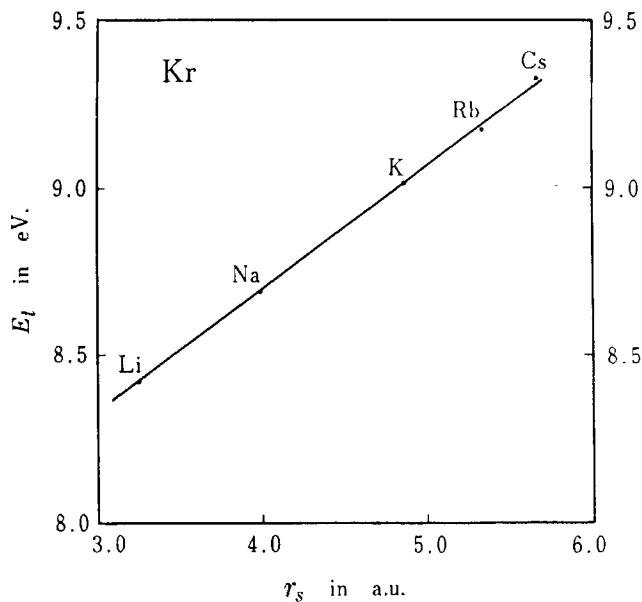


Figure 1 Threshold energy vs. interelectronic spacing r_s as observed from absorption experiments on Kr in the five alkali metals Li, Na, K, Rb and Cs.

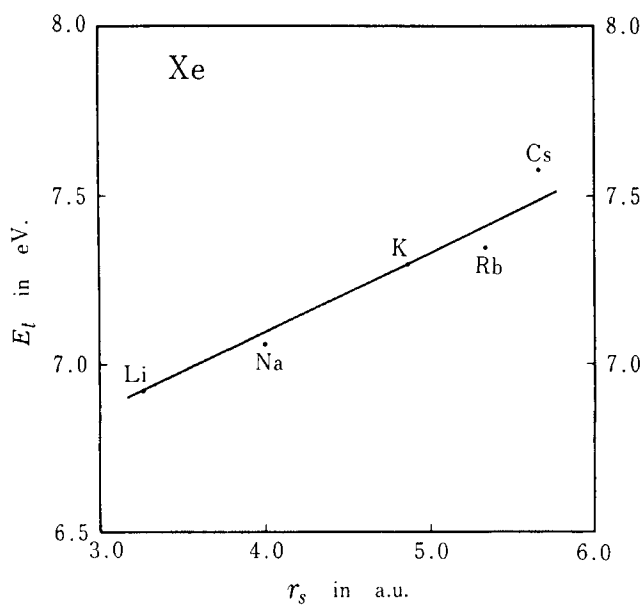


Figure 2 Same as Figure 1, but rare gas impurity is now Xe.

Table 1 Constants in linear form (1) of threshold energy E_t as function of mean interelectronic spacing r_s .

	Kr	Xe
ε_0 in eV	7.19	6.00
ε_1 in eV per Bohr radius	0.375	0.275

where Table 1 records ε_0 and ε_1 for the rare gas atoms Kr and Xe. It is tempting to modify Eq. (1) to incorporate saturation by writing

$$E_t = \frac{\varepsilon_0 + a_1 r_s + \cdots + a_n r_s^n}{1 + \left(\frac{b_1}{\varepsilon_0}\right) r_s + \cdots + \left(\frac{b_n}{\varepsilon_0}\right) r_s^n} \quad (2)$$

where evidently as $r_s/a_0 \rightarrow \infty$ we must have from the above considerations*

$$\frac{\varepsilon_0}{b_n} a_n = I. \quad (3)$$

However, we have verified that n must be greater than unity for any useful fit of the data in Figures 1 and 2 with values of I .

A further point to be considered here is the physical meaning of ε_0 and ε_1 in Eq. (1). We presume that, could the density be increased beyond the Li value the bound state of the outermost electron in the rare gas atoms would eventually give way to a virtual bound state. It seems then that, at least over a limited range of density during which all other states remain bound, the virtual bound state of the outermost electron in Kr and Xe would remain fixed at a constant separation from the Fermi level of about 6 eV for Xe and 7 eV for Kr. Of course, it will be of interest to see whether the potentials used by Ohmura *et al.*² can lead to this result, as the outermost electron enters a virtual bound state. Presumably, for the above interpretation to be reasonably precise, the width of the virtual bound state has to be a fairly small fraction of these energy separations.

* *Note added in proof*: Presumably as r_s is lowered sufficiently, one will have to consider the metal-insulator transition; specifically Wigner crystallization in the ground-state of jellium.

Two other points appear to be of potential interest in the present context:

i) He in metals has excited some interest.⁴ So far however, we know of no experimental data that will enable the analogous plot to those of Figures 1 and 2 to be made.

ii) Polyvalent metals offer, at least in principle, a way of putting points on Figures 1 and 2 at smaller r_s , down say to $r_s = 2$ for Al. But we do not presently know whether appropriate concentrations of rare gas atoms can be introduced into other metals than the alkalis.

In summary, Figures 1 and 2 can leave no doubt that the concept of rare gas atoms in a cold dense plasma is a useful one. The ideas put forward here pertaining to virtual bound states appear amenable to quantitative partial wave phase shift calculations, which are currently being planned.

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3. See for instance M. W. Cole and J. R. Klein, *Phys. Rev.*, **B35**, 8262 (1987); and K. Hoshino and A. Hasegawa, *Phys. Chem. Liquids*, **15**, 113 (1985).
4. See for example the review by M. J. Stott in *Properties of Atomic Defects in Metals*, North-Holland, Amsterdam (1978), p. 157, Eds. N. L. Peterson and R. W. Siegel.