Energy of the quasi-free electron in Argon, Krypton and Xenon

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Extraction of $V_0(\rho_P)$

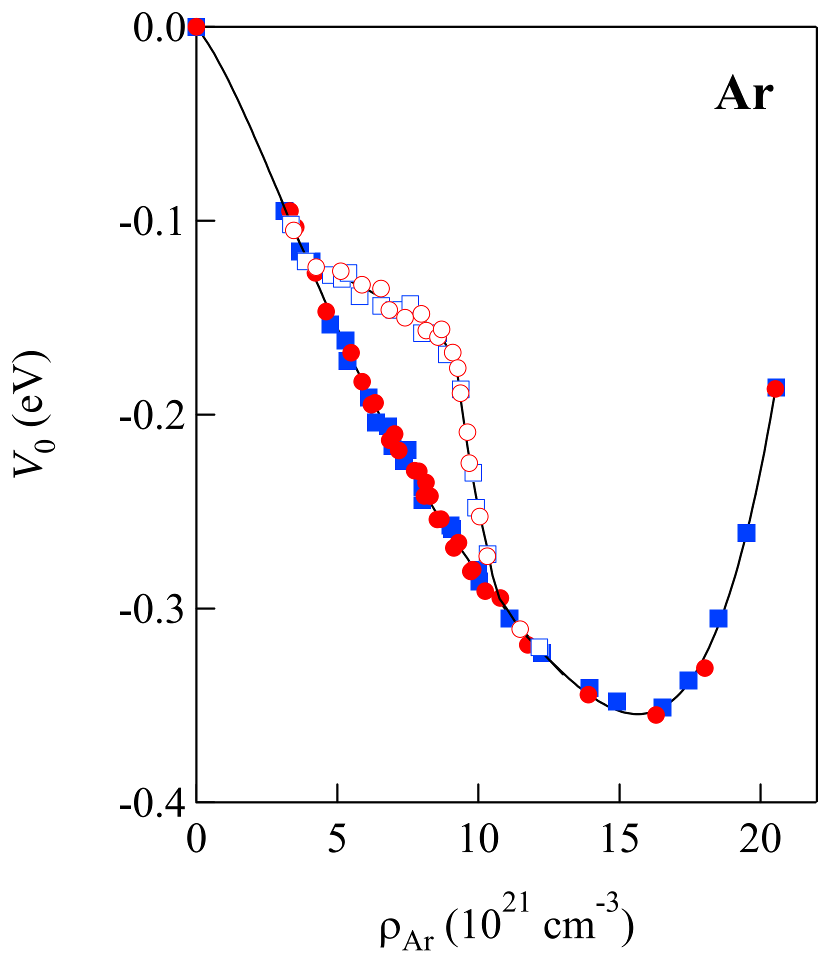
Experimental data

$$\Delta_D(\rho_P) = I_F(\rho_P) + c_0\left(\sqrt{F_L} + \sqrt{F_H}\right) - I_g$$

$$= V_0(\rho_P) + P_+(\rho_P)$$

Average ion/perturber polarization energy

$$P_+(\rho_P) = -4\pi\rho_P \int_0^\infty g_{PD}(r)\, w_+(r)\, r^2\, dr$$



Modeling $V_0(\rho_P)$

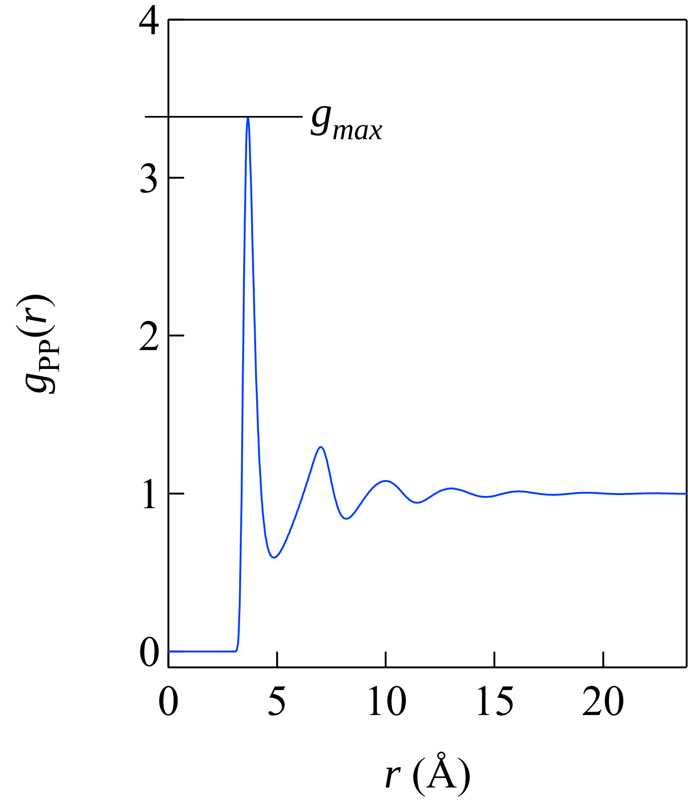
$$V_0(\rho_P) = P_-(\rho_P) + E_k(\rho_P) + \frac{3}{2} k_B T$$

Average electron/perturber polarization energy

$$P_-(\rho_P) = -4\pi\rho_P \int_0^\infty g_{PP}(r)\, w_-(r)\, r^2\, dr$$

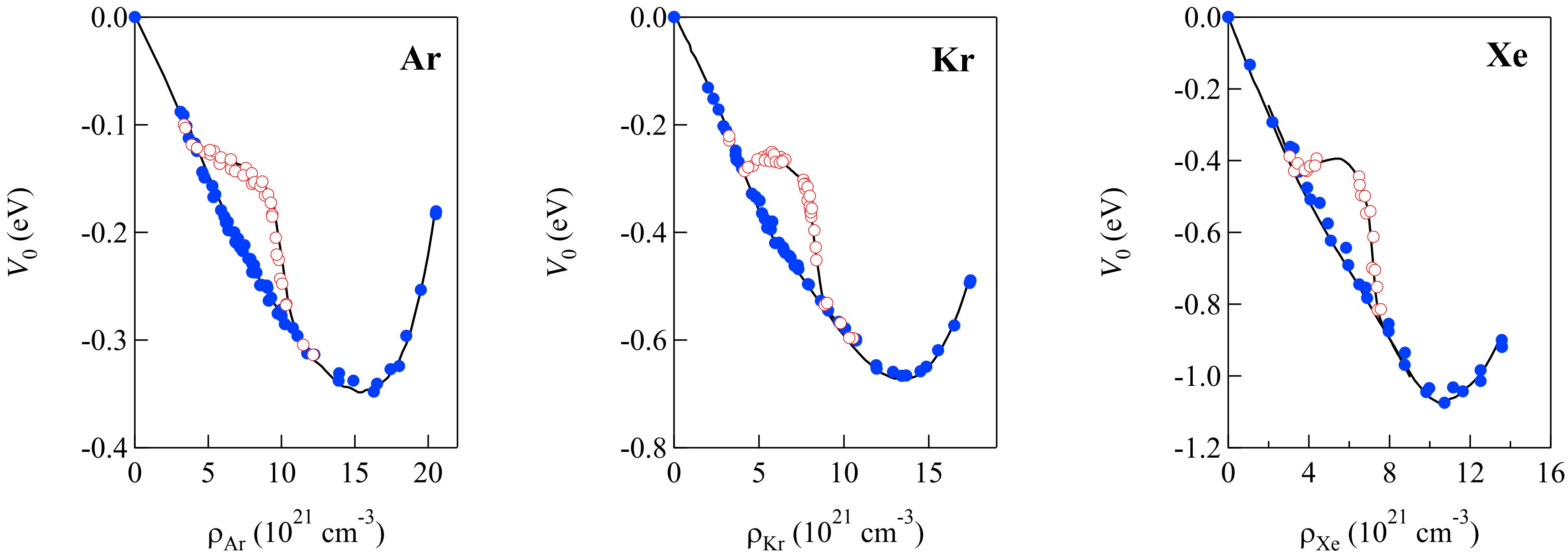
Zero point kinetic energy of the quasi-free electron

$$E_k(\rho_P) = \frac{\hbar^2 k_0^2}{2 m_e} = \frac{\hbar^2 a^2}{2 m_e} \quad \frac{1}{(r_\ell - r_h)^2} \quad , \qquad r_\ell = \sqrt[3]{\frac{3}{4\pi\, g_{max}\, \rho_P}}$$



$V_0(\rho_P)$ for Ar, Kr and Xe

Ar	Kr	Xe
$a = 0.329$	$a = 0.133$	$a = 0.0745$
$r_h = 0.820$ Å	$r_h = 1.60$ Å	$r_h = 3.24$ Å



Local Wigner-Seitz Model

The one-electron Schrödinger equation is

$$\left[-\frac{\hbar^2}{2\,m_e}\nabla^2 + V(r)\right]\psi_0 = V_0\,\psi_0$$

Assume that $V(r)$ has an average translational symmetry defined by $V(r) = V(r + r_\ell)$

The single electron potential $V(r)$ is defined as

$$V(r) = P_- + V_a(r) \quad , \qquad V_a(r) = \begin{cases} 0\,, & r > r_h \\ \infty\,, & r < r_h \end{cases}$$

Solution

$$\psi_0 = \frac{1}{r}\sin\left[k_0(r - r_h) + \delta\right]$$

$$V_0(\rho_\mathrm{P}) = P_-(\rho_\mathrm{P}) + \frac{\hbar^2\,k_0^2}{2\,m_e} + \frac{3}{2}k_B\,T \quad , \qquad \tan\left[k_0\left(r_\ell - r_h\right) + \delta\right] = k_0\,r_\ell$$

Effective Range Theory

The phase shift δ is due to perturber polarization for perturbers close to the optical electron, since $P_{-}(\rho_P)$ only accounts for the average polarization of perturbers at a distance $r >> r_{\ell}$.

The electron-atom scattering phase shift has the form

$$\tan \delta \approx A_1\, k_0 + A_2\, k_0^2 + O(k_0^3)$$

Solving the boundary condition equation for δ gives

$$\delta = \tan^{-1}\left(k_0\, r_{\ell}\right) - k_0 (r_{\ell} - r_h)$$

Phase shift dependence

$$\tan \delta \approx A_1\, k_0 + A_2\, k_0^2 + O(k_0^3)$$

Ar
$A_1 = 0.670 \pm 0.001$ Å
$A_2 = -0.031 \pm 0.005$ Å^2

Kr
$A_1 = 1.58 \pm 0.00$ Å
$A_2 = -0.300 \pm 0.008$ Å^2

Xe
$A_1 = 3.16 \pm 0.01$ Å
$A_2 = -0.577 \pm 0.006$ Å^2