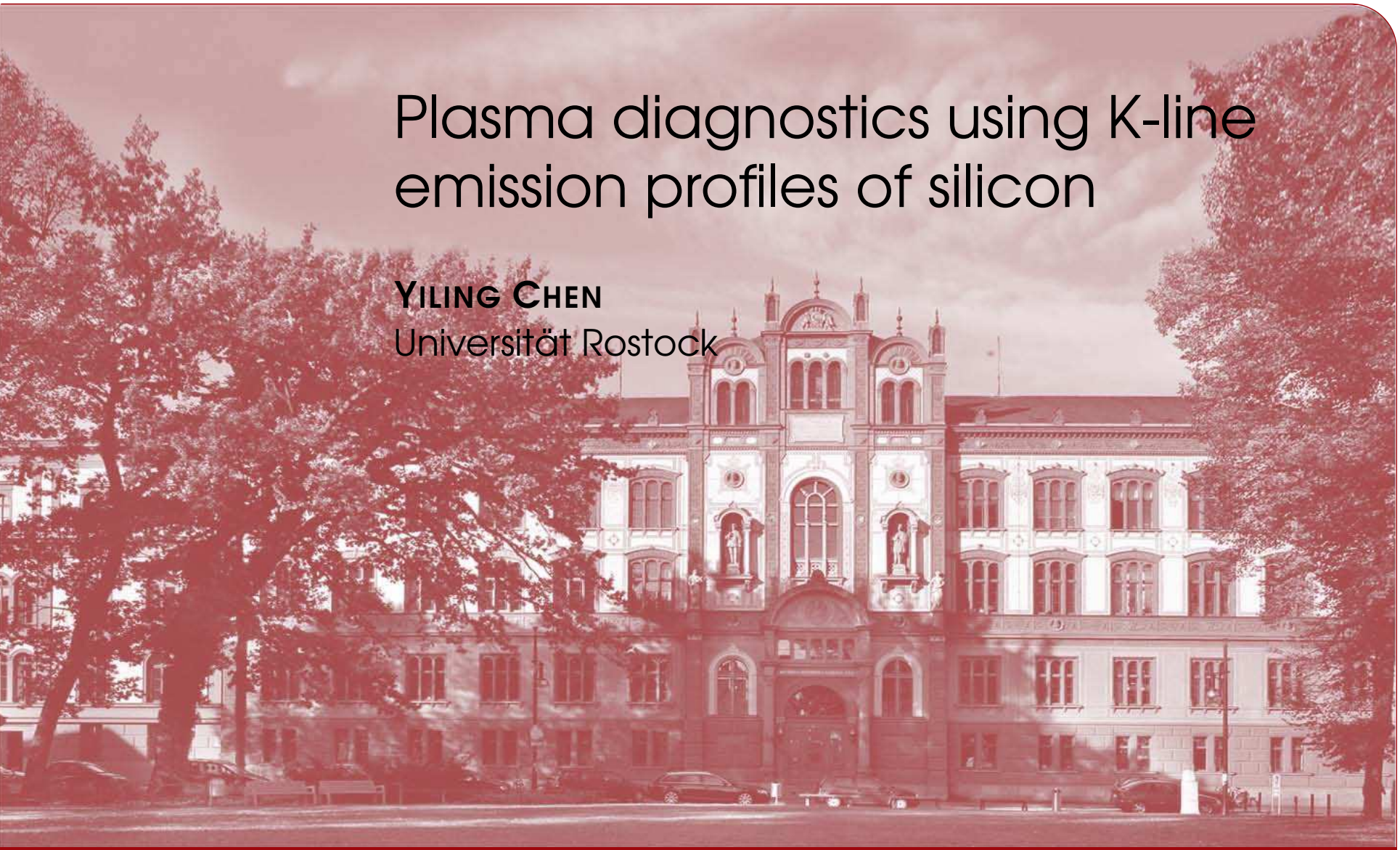
Universität Rostock

Traditio et Innovatio



Plasma diagnostics using K-line emission profiles of silicon

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Outline

Motivation

+ K_α plasma diagnostics
+ Si K_α flourescence spectra

Theory

+ Line shift due to excitation and ionization
+ Line shift due to plasma environment
+ Plasma composition

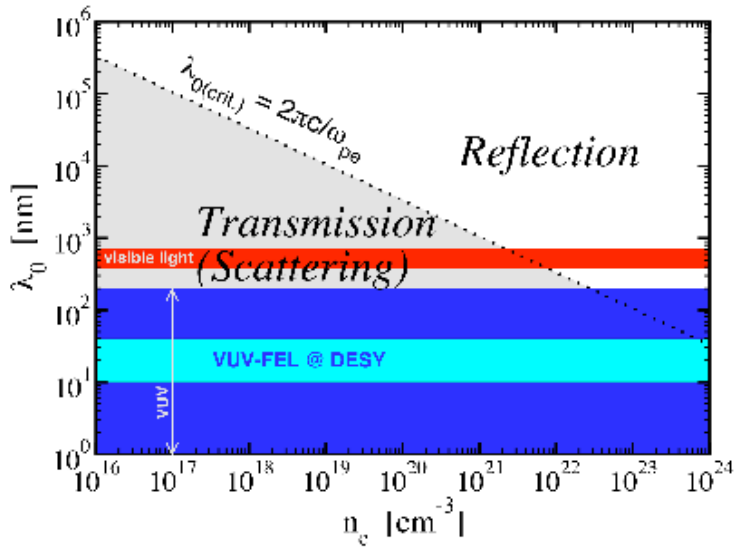
Results

+ Synthetic spectra

Summary and Outlook

K_α plasma diagnostics

+ mid-z materials K_α: in X ray range (100 eV-1 Mev) relevant for diagnostics
+ warm dense matter (n_e: $10^{20} - 10^{24}$ cm^{-3})
+ propagation in warm dense matter
+ modification of spectral line profiles.

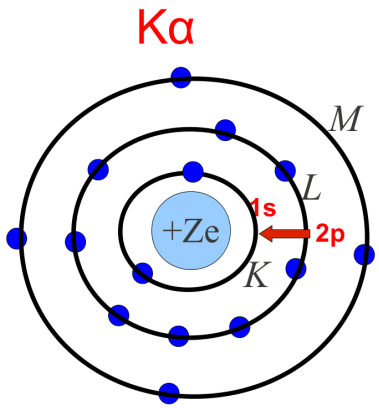


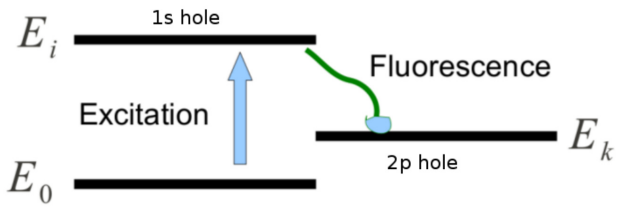
+ $\lambda = \frac{2\pi c}{\omega_{pl}}$, $\omega_{pl}^2 = \frac{n_e e^2}{\epsilon_0 m_e}$
+ reflectivity $R = |\frac{\sqrt{\epsilon}-1}{\sqrt{\epsilon}+1}|^2$
+ long wavelength limit $k \to 0$
+ $\lim_{k\to 0} \epsilon^{RPA} = 1 - \frac{\omega_{pl}^2}{\omega^2}$
+ $\omega_{pl} < \omega$, $R < 1$
+ $\omega_{pl} > \omega$, $R = 1$

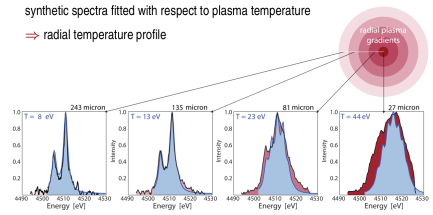
K_α emission line in flourescence spectra

Warm dense matter

+ the electron excitation from E_0 (ground state) to E_i (initial state) and photon emission from E_i to E_k (final state) in K_α fluorescence

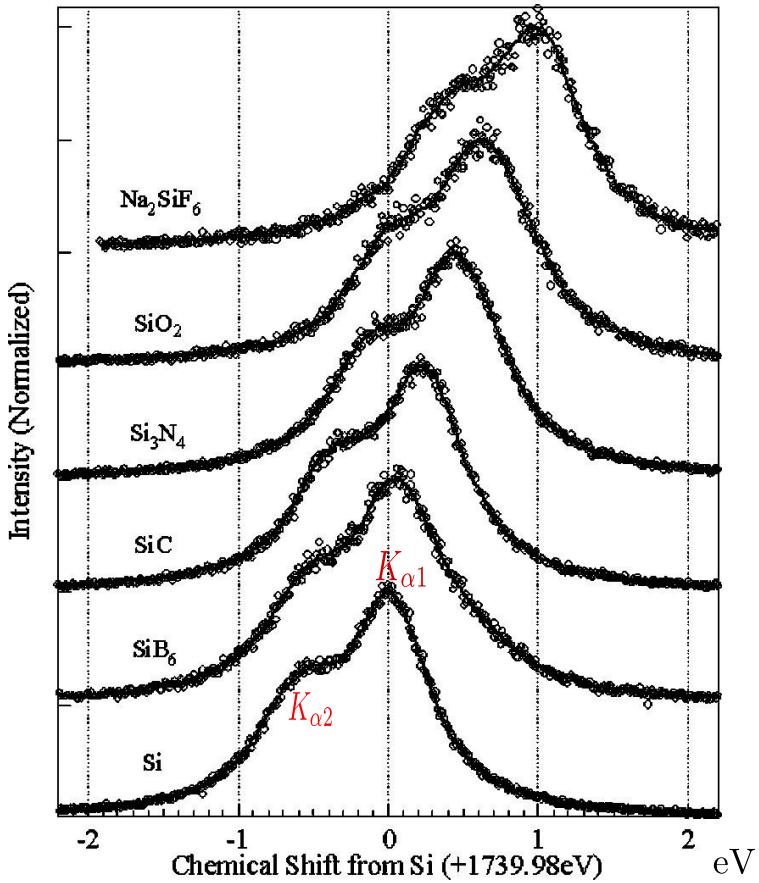






+ titanium U. Zastrau, A. Sengebusch et al,. *High Energy Density Phys. 7,47-53 (2011)*
+ Si: solid density $n_{tot} = 5x10^{22}cm^{-3}$
+ different emitter configurations are considered

Si K_α emission line in flourescence spectra



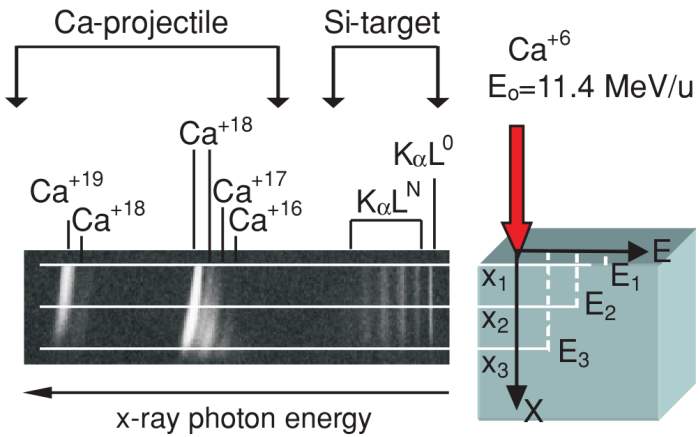
- K_α x-ray fluorescence spectra of pure Si and Si compounds
- cold emitters T $\approx$ 1 eV
- fine structure $K_{\alpha 1}$ and $K_{\alpha 2}$
- shifts due to chemical binding depending on chemical surrounding

Zhenlin Liu, Shouichi Sugata,et al., *Phys. Rev. B* ***69***, *035106 (2004)*

Si emission lines from SiO_2 aerogel

(At UNILAC accelerator at GSI-Damstadt)

+ X-ray emission spectra of low-density SiO_2 aerogel induced by Ca projectiles



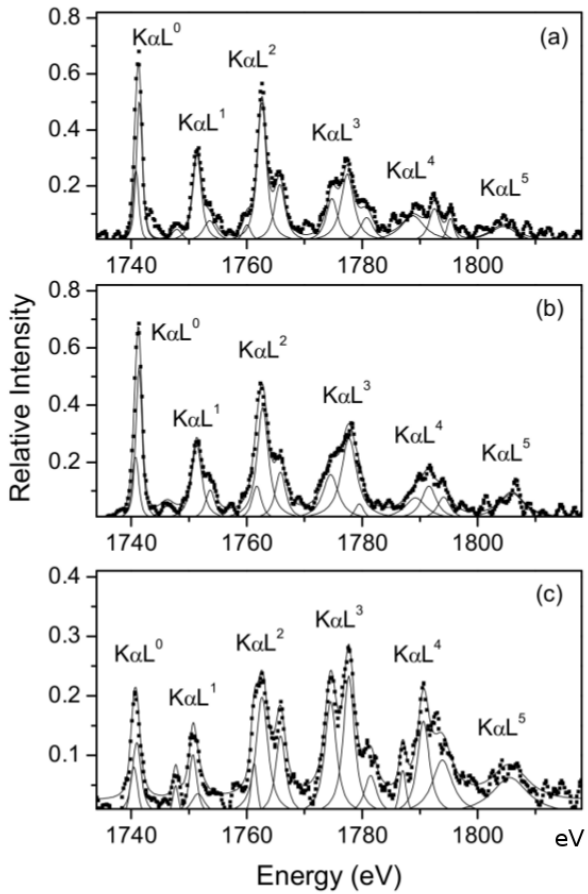
+ different penetration depths x
+ different penetration energies E

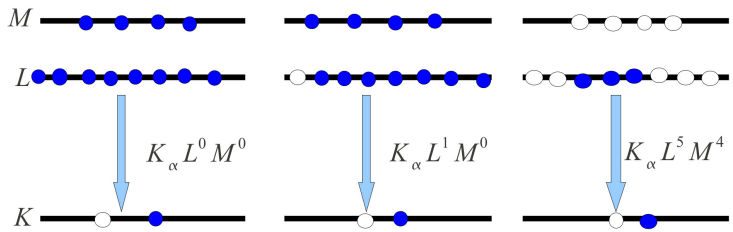
(a) x_1=0.5mm (E_1=11.4-10.6 MeV/u)
(b) x_2= 5 mm (E_2= 8.5- 7.6 MeV/u)
(c) x_3=10 mm (E_3= 5.2- 4.0 MeV/u)

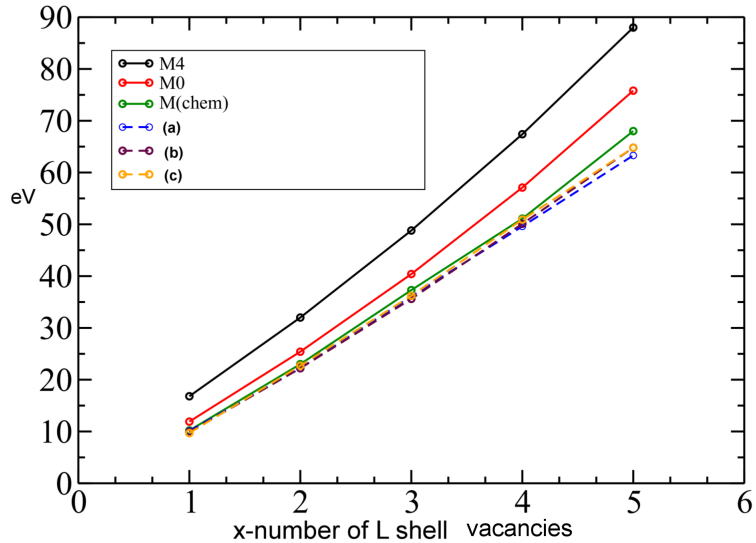
J. Rzadkiewicz, A. Gojska et al., *Phys. Rev. A* ***82****, 012703 (2010)*

Si $K_\alpha L^x M^y$ satellites, (x=N=0-5, y=0,4)

Phys. Rev. A ***82****, 012703 (2010)*







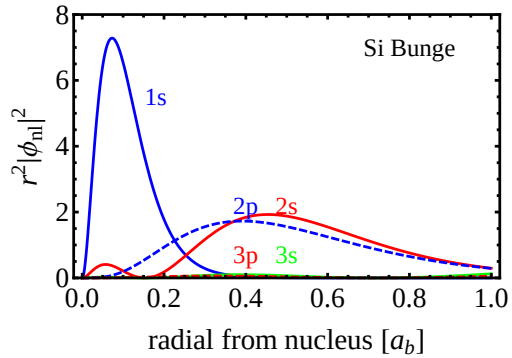
Theory- Blue shift due to excitation and ionization

+ description of isolated ionic emitter H^0 by self-consistent

Roothaan – Hartree – Fock equations. C. C. J.Roothaan (1951).

+ Bunge wave function $\phi_{nlm}(r,\theta,\phi) = R_{nl}(r) \cdot Y_{lm}(\theta,\phi)$

$$R_{nl} = \sum_j S_{jl} C_{jln}$$

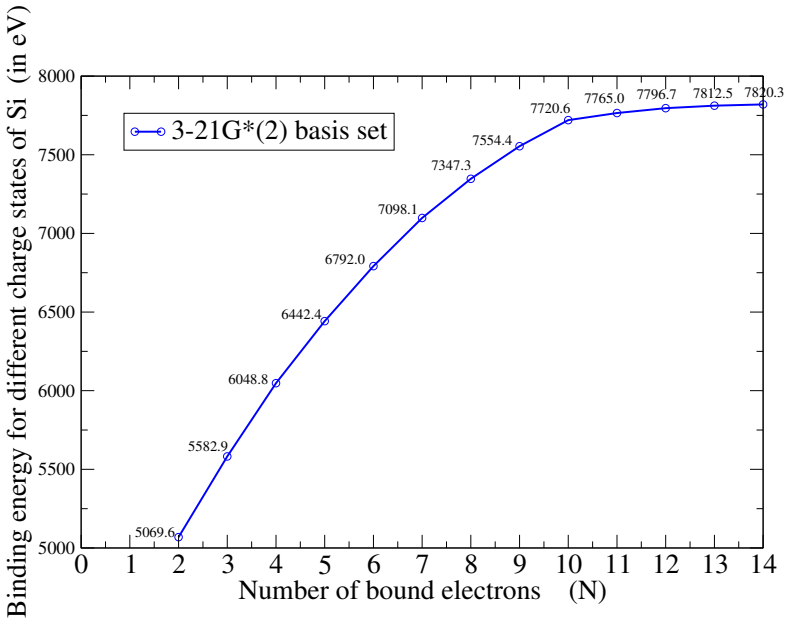


+ Gaussian wave function H. B. Schlegel and M. J. Frisch, *International Journal of Quantum Chem. 54, 83-87 (1995).*

$$G_g(\vec{r}, l_x, l_y, l_z, \alpha) = N(l_x, l_y, l_z, \alpha) x^{l_x} y^{l_y} z^{l_z} e^{-\alpha \vec{r}^2}$$

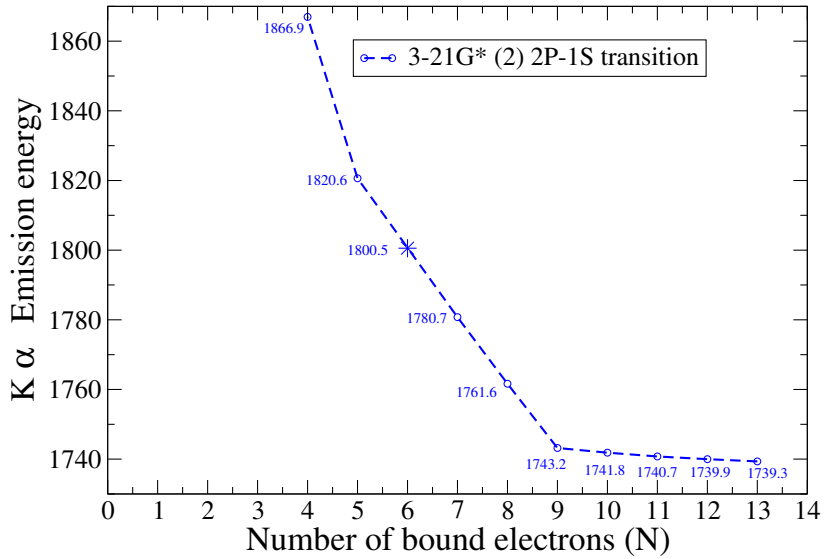
+ unperturbed ionization and emission energies obtained from chemical *ab initio* code G03
+ using Gaussian basis set: $3-21\mathrm{G}^*$, 19 basis functions

Binding energy



+ Ground state of Si:
  $1s^2 2s^2 2p^6 3s^2 3p^2$

K_α emission energy



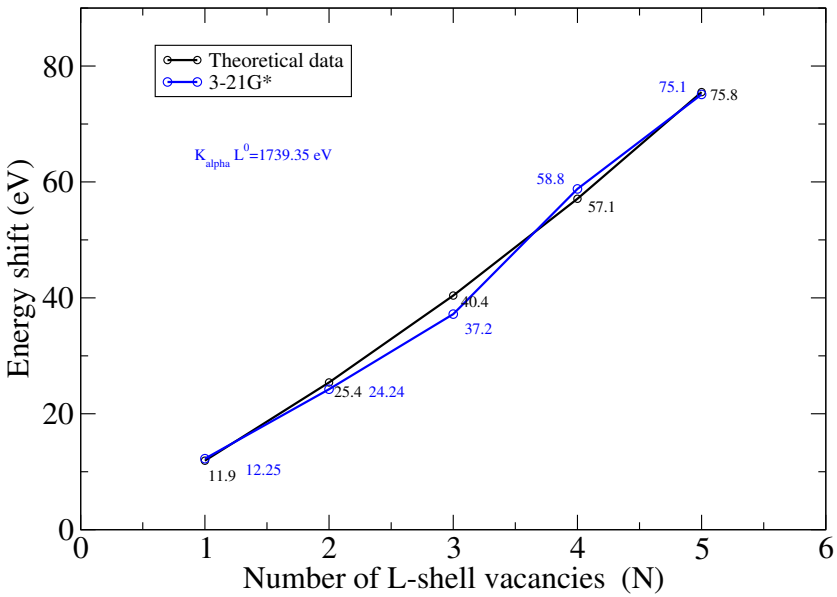
+ for emission of Si^+ (N=13):
  initial state: $1s^1 2s^2 2p^6 3s^2 3p^2$
  final state: $1s^2 2s^2 2p^5 3s^2 3p^2$

$K_\alpha L^N M^0$ and $K_\alpha L^N M^4$

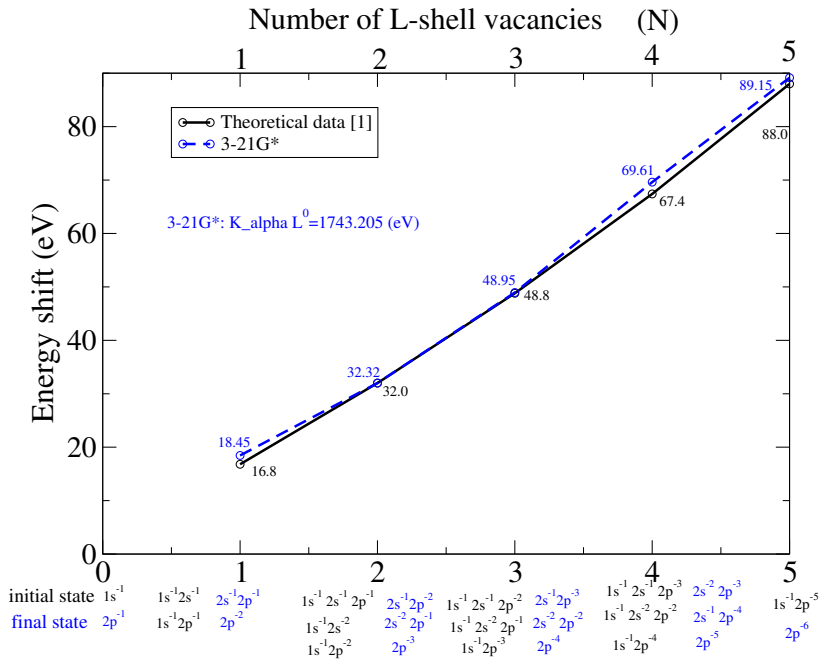
Comparison of the $K_\alpha L^0$ with satellites energy shifts

$K_\alpha L^N M^0$

M0: represents the ground-state $3s^2\ 3p^2$



$K_\alpha L^N M^4$



Theoretical data: J. Rzadkiewicz, A. Gojska et al., *Phys. Rev. A* ***82****, 012703 (2010)*

Red shift due to plasma polarization

+ Ion sphere potential obtained from Poisson-equation :

$$\Delta\phi(r) = 4\pi e\, n_{\mathrm{f}}(r) + 4\pi e\, n_{\mathrm{b}}(r) - 4\pi Ze\, \delta(r)$$

+ density of bound electrons: $n_b = \frac{1}{4\pi} \sum_{nl} |R_{nl}(r)|^2$

+ self-consistency with respect to free electron density:

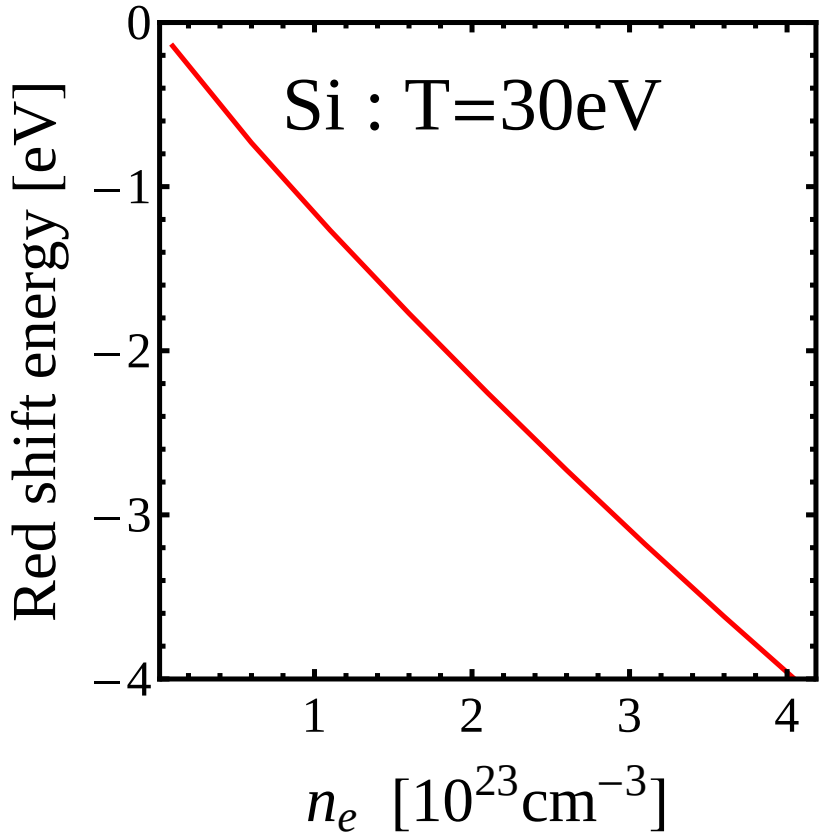
$$n_{\mathrm{f}}(r) \propto \int_{p_0}^{\infty} \frac{dp\, p^2}{(2mk_B T)^{3/2}} \exp\left[\left(\frac{-p^2}{2mk_B T} + \frac{e\,\phi(r)}{k_B T}\right)\right],\ p_0 = \sqrt{2me\phi(r)}$$

+ perturbative ansatz $H = H^0 + H'$ with $H' = -e[\phi(r) - \phi(r, n_{\mathrm{f}} = 0)]$

+ due to plasma shift energies polarization due to plasma screening:

$$\Delta E^{(1)} = < \psi_i | H' | \psi_i > - < \psi_f | H' | \psi_f >$$

Red shift due to plasma polarization



+ using Bunge RHF function
+ configuration of Si^+ :

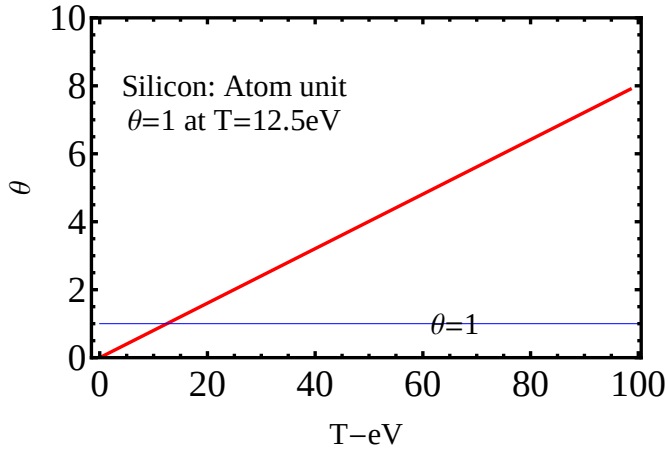
initial state :
$1s^1 2s^2 2p^6 3s^2 3p^2$

final state :
$1s^2 2s^2 2p^5 3s^2 3p^2$

Plasma Composition

Coupled saha equation

+ Degeneracy parameter $\Theta = \frac{k_B T}{E_{\mathrm{Fermi}}} > 1,\ E_{\mathrm{Fermi}} = \frac{\hbar^2}{2m_e}(3\pi^2 n_e)^{2/3}$
+ Boltzmann distribution function $f_e(p) = e^{-\beta(p^2/2m_e - \mu_e)}$
+ due to relations $\mu_m = \mu_{m+1} + \mu_e$ assuming local thermal equilibrium conditions
+ iteration to be solved : $n_{(m)} = \left[e^{-\mu_e/k_B T}\right]^m \frac{\sigma^{in}_{(m)}}{\sigma^{in}_{(0)}} n_{(0)}$



electron-ion interaction

+ Wigner-Seitz radius R defined by $R = \left(\frac{Z_{ion}}{4\pi n_e}\right)^{1/3}$
+ the ion sphere has Wigner-Seitz radius R to build ion-electron shift :

$$\Delta_e^{ei} = -\frac{Z_{ion}e^2}{4\pi\epsilon_0 R} = -\frac{e^2}{\epsilon_0}\left(\frac{Z_{ion}}{4\pi}\right)^{2/3}\left(\frac{n_e}{3}\right)^{1/3}$$

+ internal partition function of ion-electron shift:
  (m: number of ionisation steps)

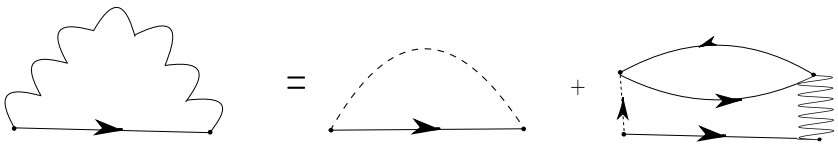
$$\sigma_e^{in}(m) = 2^m exp\left[\frac{1}{k_b T}\frac{e^2}{(4\pi)^{2/3}\epsilon_0}\left(\frac{n_e}{3}\right)^{1/3}\sum_{x=1}^{m} x^{2/3}\right]$$

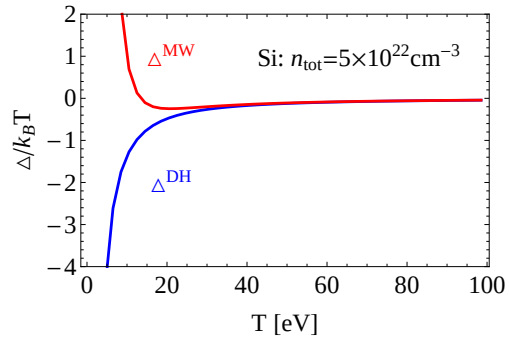
electron-electron interacton

+ then the electronic chemical potential in the classical low density case reads

$$\mu_e = \frac{n_e\lambda_e^3}{2} - \frac{e^2}{2}\sqrt{\frac{n_e e^2}{\epsilon_0 k_B T}} + \frac{\sqrt{2\pi^2}\, n_e \lambda_e e^4}{8(k_B T)^2} - \frac{n_e\lambda_e^3}{8\sqrt{2}} + \frac{n_e\lambda_e^2 e^2}{4 k_B T}$$

+ Montroll-Ward approximation: $= \Delta^{HF} + \Delta^{MW}$





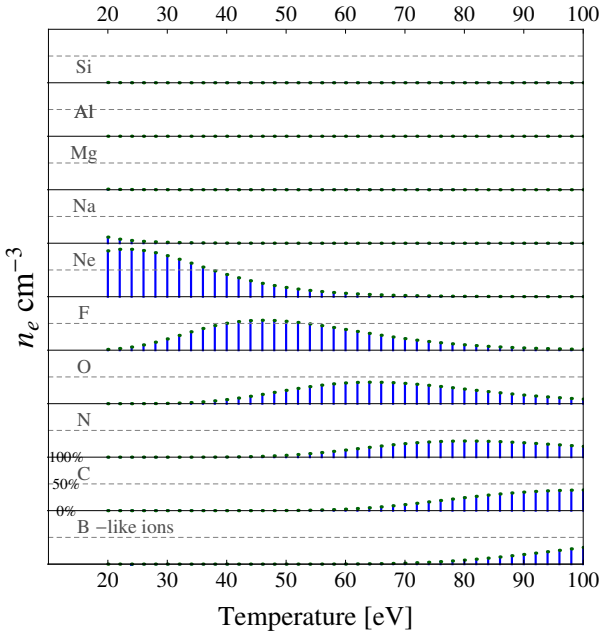
Plasma Composition

Planck-Larkin partition function

+ $\sigma_e^{in}(m) = 2^m \exp\left[-\frac{\Delta_e^{MW}}{k_B T}\right]^m \exp\left[\frac{1}{k_B T}\frac{e^2}{(4\pi)^{2/3}\epsilon_0}\left(\frac{n_e}{3}\right)^{1/3}\sum_{x=1}^{m} x^{2/3}\right]$

+ Planck-Larkin partition function for bound contributions

$$\sigma^{in,PL} = \sum_{nl}(2l+1)\left(\exp\left[-\frac{E_{nl}}{k_B T} - 1\right] + \frac{E_{nl}}{k_B T}\right)$$



Synthetic spectra

+ average emission power from N_i atoms in state E_i

$$\langle P \rangle_{ik} = N_i \cdot A_{ik} \cdot \hbar \cdot \omega_{ik}$$

+ with spontaneous transition probability,

$$A_{ik} = \frac{2e^2\omega_{ik}^3}{3\epsilon_0 c^3 h} \left| \frac{1}{\Omega_0} \int \psi_i^* \vec{r} \psi_k d^3 r \right|^2$$

+ with approximation

$$\langle P \rangle_{ik} = N_i E_0 A$$

+ intensity give as

$$\frac{I_{max}}{I_{ref}} = \frac{N_i E_0 A}{N_{ref} E_0^{ref} A_{ref}} \simeq \frac{n}{n_{ref}} \left(\frac{E_0}{E_0^{ref}} \right)^4$$

Synthetic spectra

+ Lorentz profil for individual spectral lines

$$I_{Lorentz}(E) = \frac{I_{max}(\gamma/2)^2}{(E - E_0)^2 + (\gamma/2)^2}$$

+ convoluted with Gaussian instrument function

$$I(E) = \int_{-\infty}^{\infty} dz\ I_{Lorentz}(E + z) \frac{1}{\sqrt{2\pi\Gamma_G^2}} \exp\left[-\frac{z^2}{2\Gamma_G^2}\right]$$

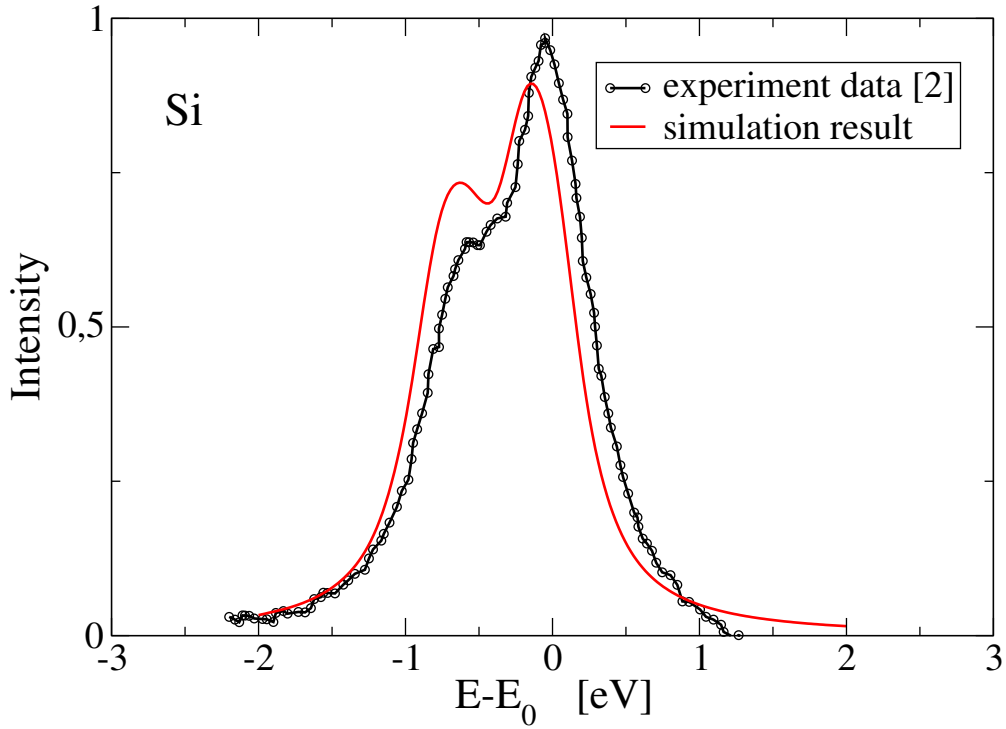
+ fixed parameters for Si:

  Lorentzian linewidth $\gamma = 0.43$ eV
  Gaussian width $\Gamma_G = 0.13$ eV

G.Graeffe, H. Juslen et al., *J.Phys. B: Atom. Molec. Phys., Vol. 10, No. 16,1977*

$K_\alpha L^0 M^0$ line for Si

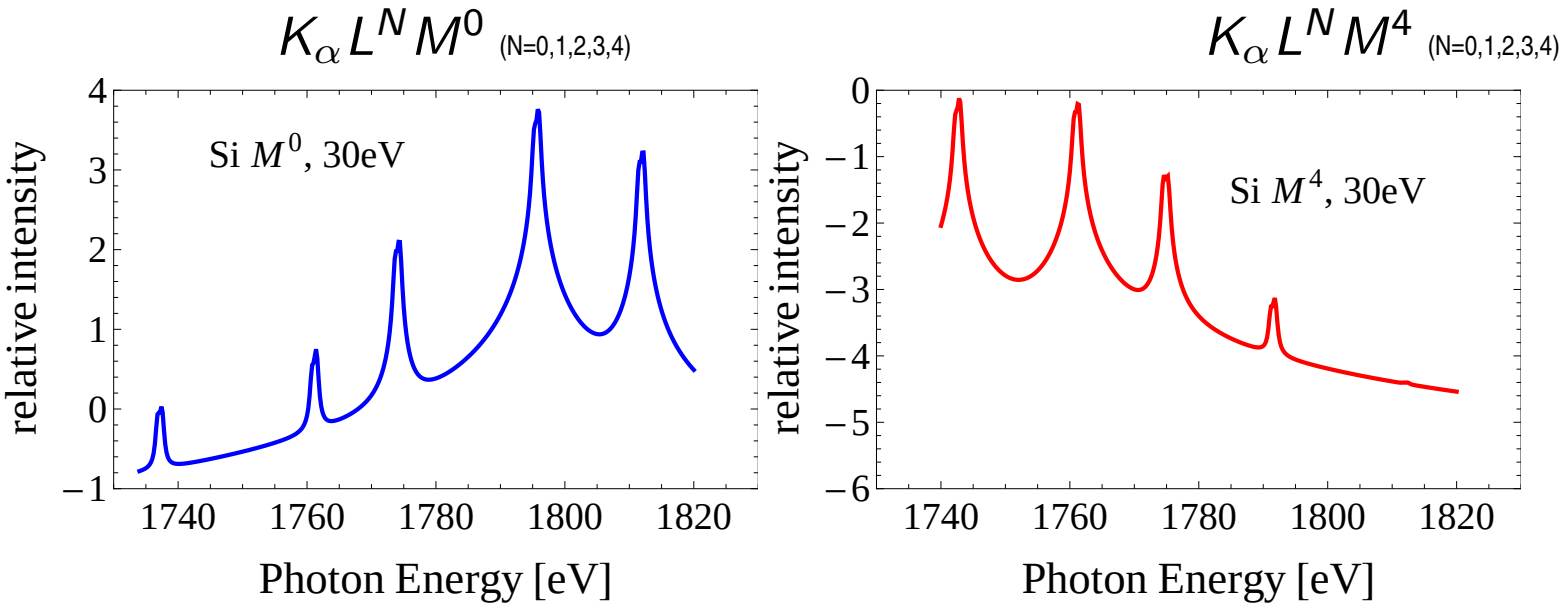
T= 30 eV, $n_{tot} = 5x10^{22} cm^{-3}$



+ fine structure $P_{3/2}$ and $P_{1/2}$ influence the intensity
+ distance of 0.591 eV between fine-structure components (semi-empirical NIST data)
+ experiment data [2]: Zhenlin Liu, Shouichi Sugata,et al., *Phys. Rev. B* ***69****, 035106 (2004)*

spectrum with satellite emission lines

temperature = 30 eV



Summary and Outlook

+ X-ray emissions strongly depend on the ion configuration and emitter environment
+ red and blue energy shifts are determined by emitter configuration and plasma parameters
+ spectra with different temperatures
+ the photon emission spectra are considered using different configurations to improve M^0 for the x-ray transitions in $K_\alpha L^N$ satellites

thank you

background: http://3.bp.blogspot.com/__PImM2TTud6Y/SsNv3CM9mEI/AAAAAAAABxY/lNvsuM6tzsc/s1600-h/20090618-2039.jpg

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God, My parents, Heidi Reinholz, Gerd Röpke, Olga Rosmej, Jacek Rzadkiewicz, Andrea Sengebusch, Sonja Lorenzen, Thmoas Keil, Volker Mosert, Niels-Uwe Bastian, SFB652