Научно-координационная Сессия
"Исследования неидеальной плазмы"

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УСТОЙЧИВОСТЬ КРИСТАЛЛА LiF В РАЗОГРЕТОМ ПЛОТНОМ СОСТОЯНИИ

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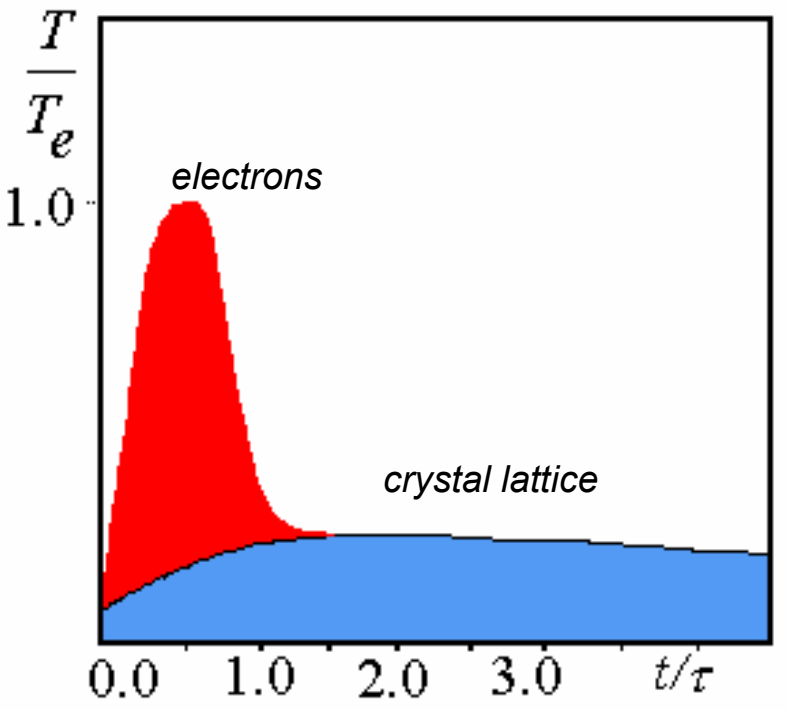
ОИВТ РАН

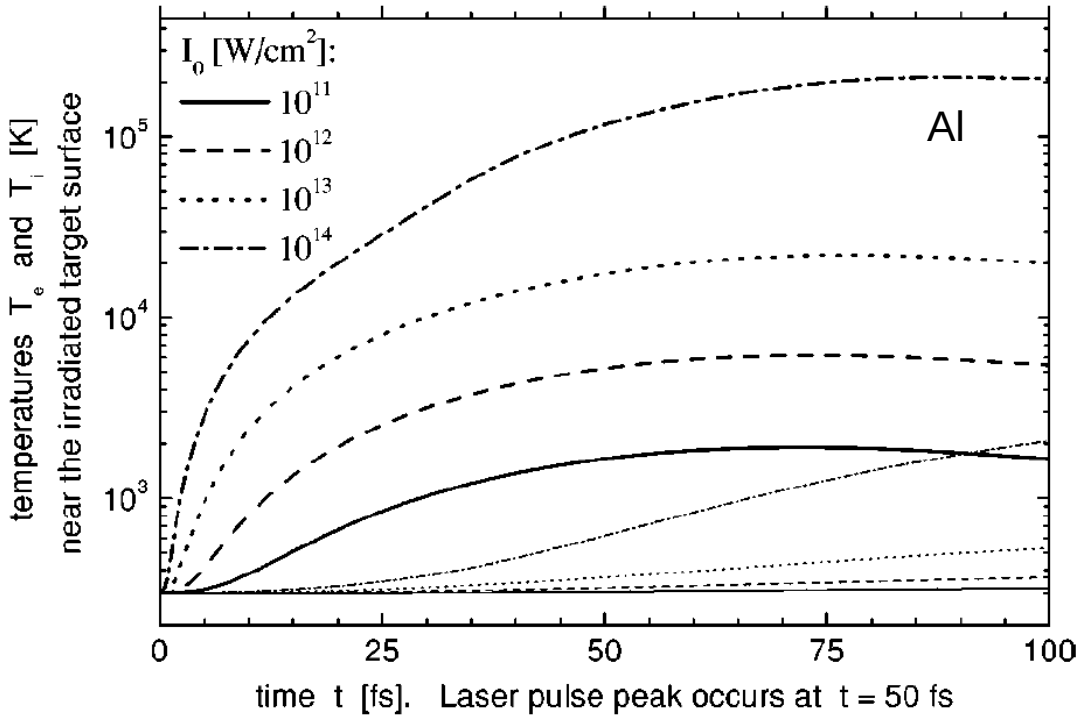
МФТИ

Influence of the electronic system excitation on crystal lattice stability

Dynamics of the crystal lattice after femtosecond pulse irradiation

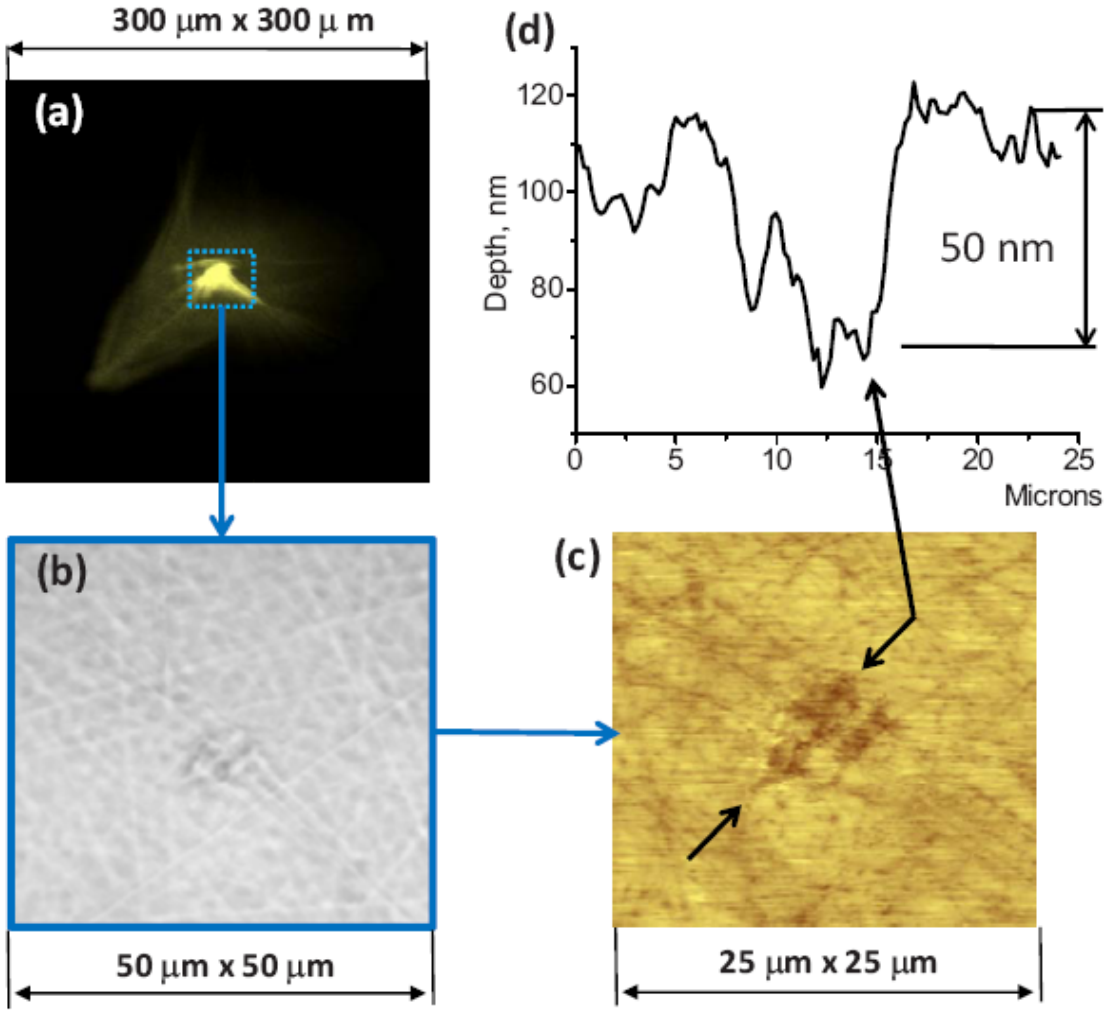
Two-temperature system
«cold» lattice – hot «electrons»





Fisher et al., 2001

Low-threshold ablation of dielectrics irradiated by picosecond soft x-ray laser pulses



A. Yu. Faenov et al., Appl. Phys. Lett., vol. 94, p. 231107, 2009

Electronic density functional theory

Density Functional Theory

N-electron wave function

$$\Psi(\vec{r}^{\,N})$$

$\Downarrow$ Hohenberg-Kohn theorem

One-electron density

$$n(\vec{r})$$

$\Downarrow$ Kohn-Sham scheme

N one-electron orbitals

$$\Phi_1(\vec{r}),\ldots,\Phi_N(\vec{r})$$

Connection:

$$N\int d\vec{r}_2 \ldots d\vec{r}_N \left|\Psi(\vec{r},\vec{r}_2 \ldots \vec{r}_N)\right| = n(\vec{r}) = \sum_{i=1}^{N} \left|\Phi_i(\vec{r})\right|^2$$

Density Functional Theory

$$E[n] = T_s[n] + V_H[n] + E_{xc}[n] + \int d\vec{r}\, n(\vec{r}) v(\vec{r})$$

$$T_s[n] = -\frac{1}{2}\sum_{i=1}^{N} \left\langle \Phi_i \left| \nabla^2 \right| \Phi_i \right\rangle$$

$$\left(-\frac{1}{2}\nabla^2 + \frac{\delta V_H[n]}{\delta n(\vec{r})} + \underbrace{\frac{\delta E_{xc}[n]}{\delta n(\vec{r})}} + v(\vec{r}) \right) \Phi_i = \varepsilon_i \Phi_i$$

approximations to the exchange-correlation term
LDA, GGA etc.

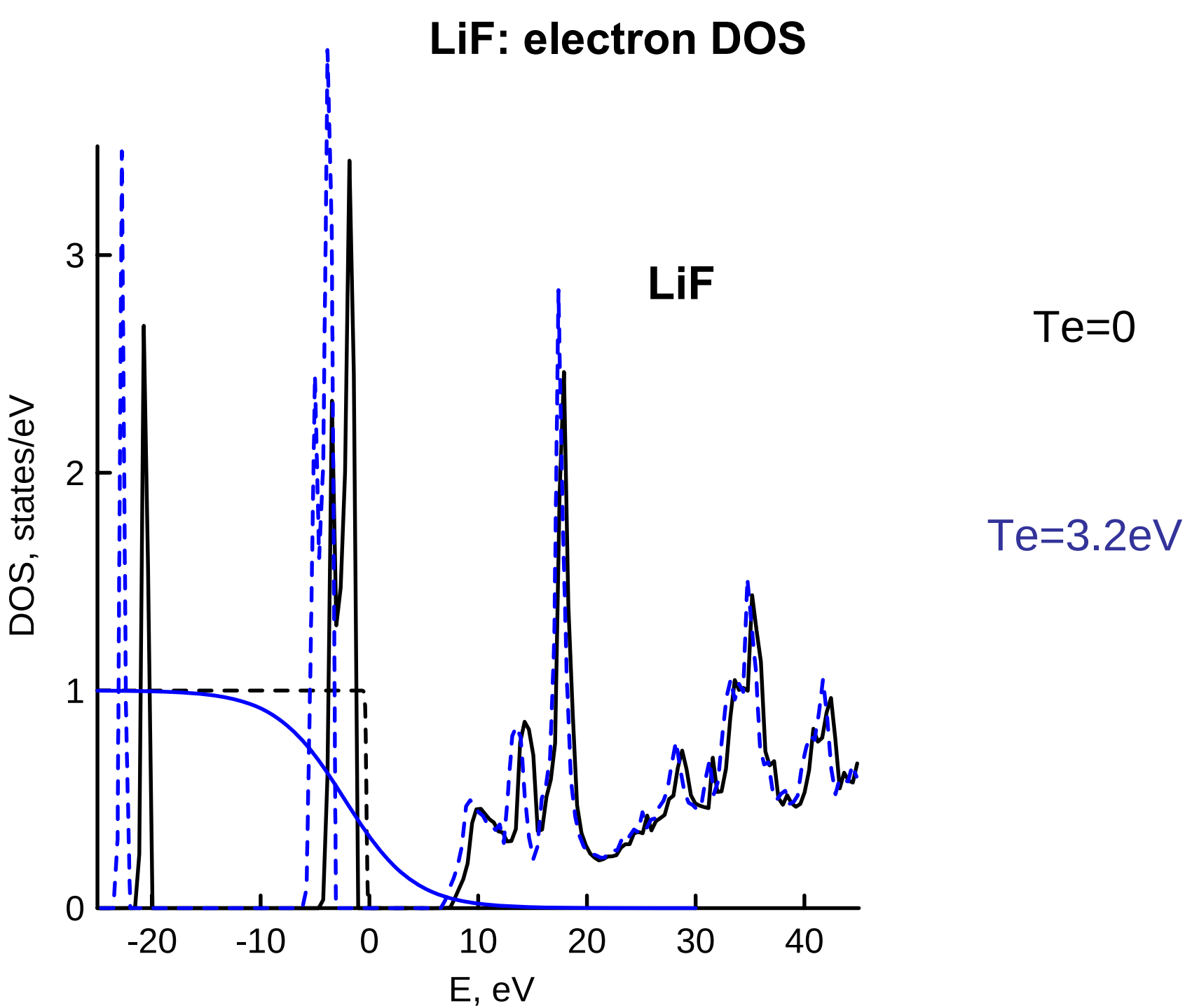
T>0: Mermin functional

$$f_i(\beta) = \frac{1}{1+\exp\left[\beta\left(\varepsilon_i - \mu\right)\right]}$$

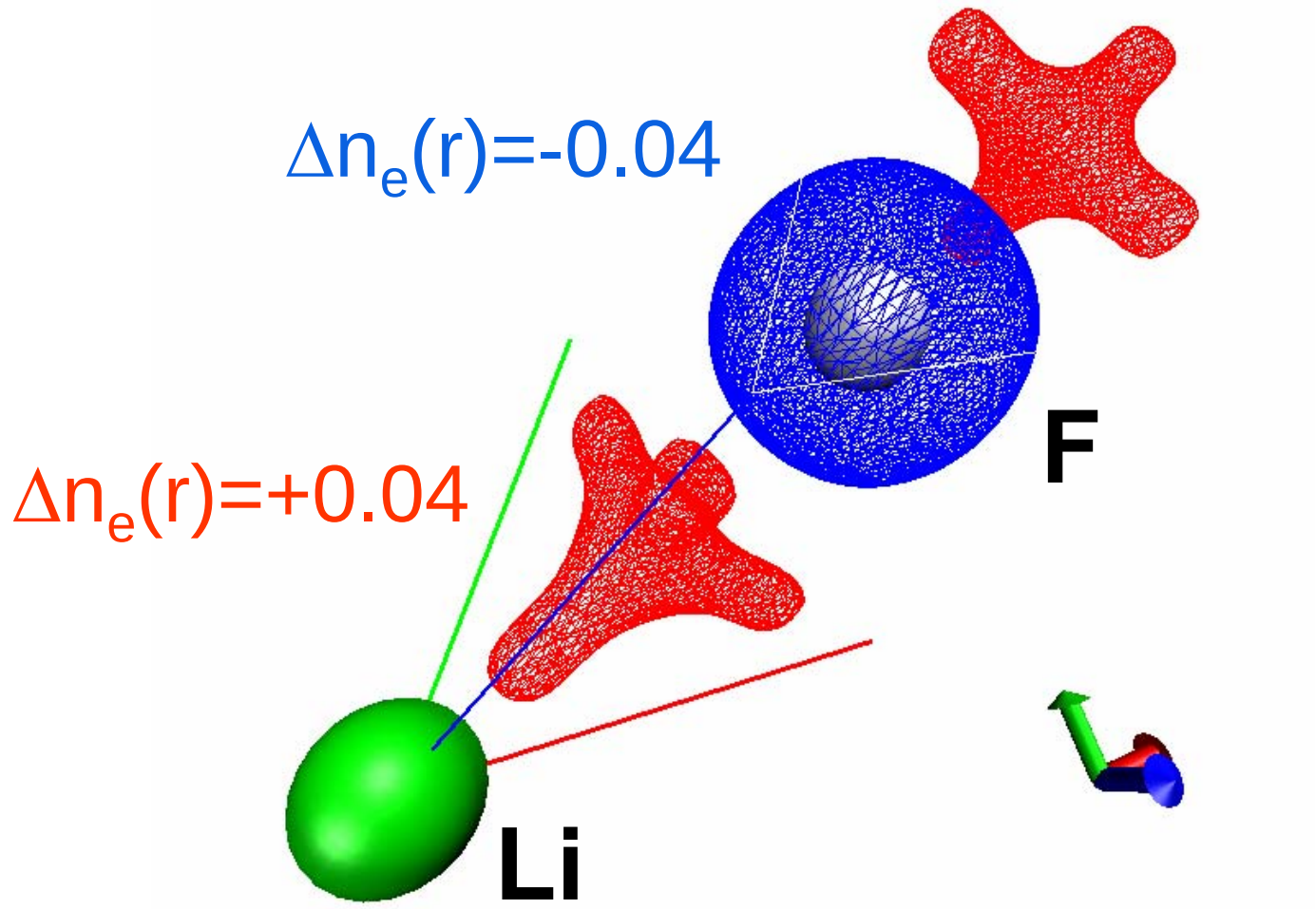
$$n(\vec{r}) = \sum_{i=1}^{N} f_i(\beta)\left|\Phi_i(\vec{r})\right|^2$$

$$\Omega[n] = T_s[n] + V_H[n] + \Omega_{xc}[n] + \int d\vec{r}\, n(\vec{r})v(\vec{r})$$

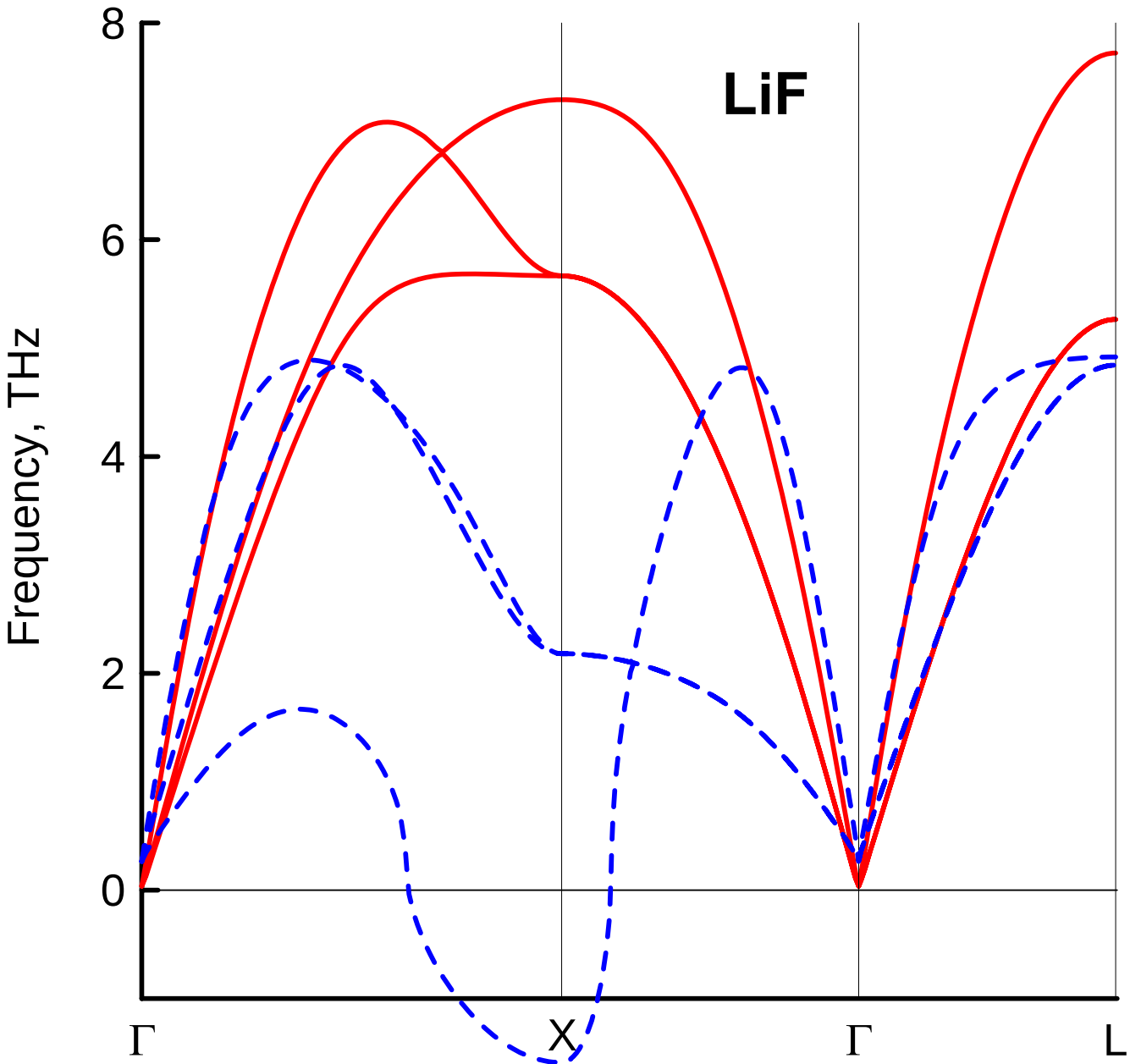
Mermin, 1965


LiF: electron DOS
LiF
Te=0
Te=3.2eV
DOS, states/eV
E, eV
0
1
2
3
-20
-10
0
10
20
30
40

Redistribution of the electron density due to the heating of the electron subsystem in the LiF crystal unit cell



Phonon dispersion in LiF



Te=2.0eV

Te=3.2eV

Conclusions

The excitation of the electronic subsystem results in the loss of mechanical stability of the fcc LiF lattice that is manifested as an appearance of the soft acoustic phonon mode. The corresponding redistribution of the electronic density implies that the originally strongly ionic interatomic interaction becomes more of covalent character with the rise of electronic temperature.