Screening Dependence Study of Electronic Structure of Liquid Alkali Metals

S. N. Desai[1], I. H. Chaudhary[1], and A. M. Vora[2]

[1]Department of Physics, B. V. Shah (Vadi Vihar) Science College, C. U. Shah University, Wadhwan City 363030, Gujarat, India

[2]Department of Physics, University School of Sciences, Gujarat University, Ahmedabad 380009, Gujarat, India

Abstract

Well known model pseudopotential of in the second-order perturbation theory is used to study the electronic structure viz. electron dispersion relation, the Fermi energy and deviation in the Fermi energy from free electron value for the liquid alkali metals. The screening influence of the five different forms of the local field correction functions on the aforesaid electronic properties of liquid alkali metals is studied explicitly, which reflects the varying effects of screening and found suitable for the present study. The depth of the first negative hump in the electron dispersion of liquid alkali metals go to Li→Cs increases while positive first peak of the dispersion curves go to Li→Cs decreases.

1.   Introduction

During the several decades, considerable theoretical development taken place in the field of disordered condensed matter physics. Generally, in this field the disorder means it is a periodic random structure. The few examples of this system are crystals with impurities, liquid metals, binary alloys, metallic glasses, etc. The disordered materials are also known as non-crystalline materials. Such a liquid exhibits metallic as well as fluid-like behaviour and hence can help to make a link between the theory of the liquid states and the theory of the electronic states in metals. Therefore, the study of electronic structure properties of liquid metals and their alloys remain one of the favourite scopes either experimentally or theoretically [1-8]. The pseudopotential based investigation of the Fermi surface and its distortion from free-electron value for the metals in the solid phase are quite often and well recognized. Very recently, we have also reported successfully, the Fermi surface distortion (FSD) and Fermi energy (FE) of the solid-solutions [9, 10] and of liquid metals and their alloys [4, 5]. However, the attempts of studying the Fermi energy and its deviation form free-electron value for liquid metals are very rare [4-8].

Therefore, in the present article, an interesting task is taken up to investigate the electron dispersion relation, Fermi energy and deviation in the Fermi energy from free-electron value for liquid alkalis based on our well recognized model potential [9, 10]. The theoretical structure factors of liquid alkalis are calculated from Percus-Yevic (PY) hard sphere model with proper packing density [11]. The screening effects are also studied from the influence of five different types of the local field correction functions given by Hartree (H) [12], Taylor (T) [13], Ichimaru-Utsumi (IU) [14], Farid *et al.* (F) [15] and Sarkar *et al.* (S) [16].

2.   Theoretical Methodology

The electronic structure of liquid alkalis using the pseudopotential theory and second-order perturbation theory is written as [4-8].

$$E(k) = E_0(k) + E_1(k) + E_2(k).$$ (1)

Where, the terms $E_0(k)$, $E_1(k)$ and $E_2(k)$ are described briefly in [4-8]. Hence the deviation in the Fermi energy ΔE_F from free-electron value at the Fermi level is given by [4-8]

$$\Delta E_F = \Delta(k_F)\big|_{k=k_F} - \Delta(0)\big|_{k=k_F}.$$ (2)

Where, E_F, k_F, Z and $W(q)$ are the Fermi energy, Fermi wave vector, valence and model pseudopotential, respectively. In the present computation of the electronic structure of liquid alkalis, we have adopted our well recognized model potential [9, 10] including five different types of the local field correlation functions [12-16] are used to study the screening influence on the aforesaid properties.

3.   Results and discussion

The input parameters and other constants used in the present computations are narrated in the Table 1 and which are taken from [4, 5]. The Fermi energy at the Fermi level of liquid alkalis are narrated in Table 2.

It is seen from Table 2 that, the present results of the Fermi energy at the Fermi level of the liquid alkalis are found in qualitative agreement with available theoretical data [4-8]. Also, it is noted that, among the five local filed correction functions, the T-local field correction function provides the minimum value of the Fermi energy at the Fermi level, while those from the H- local field correction function (without exchange and correlation) provides the maximum value. It was also concluded that among all the alkalis, minimum deviation in the Fermi energy at Fermi level is obtained for liquid Li and the maximum for liquid Cs. In comparison with the static H-function, the percentile influences of various local field correction functions on the Fermi energy at Fermi level are found for Li, Na, K, Rb and Cs liquid alkalis are of the order of 0.48%-2.07%, 0.81%-3.64%, 1.41%-6.62%, 1.93%-9.30% and 2.38%-11.72% for T, IU, F and S, respectively.

The electron dispersion relations for liquid alkalis are shown in Figures 1–5. It is seen that, the negative hump observed around $k = 1.40\text{Å}^{-1}$, 1.11Å^{-1}, 0.92Å^{-1}, 0.85Å^{-1} and 0.81Å^{-1} for all the five alkalis viz. Li, Na, K, Rb and Cs, respectively. Also, the higher negative hump is observed for T-function, while those obtained for H-function is lower. As we move from Li→Cs, the magnitude of the first positive peak decreases and the positions of this peak also move towards lower wave vector. The positive peak of the dispersion curves are observed around $k = 1.04\text{Å}^{-1}$, 0.85Å^{-1}, 0.66Å^{-1}, 0.62Å^{-1} and $0.0.59\text{Å}^{-1}$ for all the five alkalis, respectively

The largest negative hump is observed for Cs element while for Na, lower hump is observed. For Li, the negative hump is not seen. Also, for the system of higher atomic mass and atomic volume, the influence of exchange and correction function is found more. The influence of various local-field correction functions is clearly visible for higher values of wave vector. The exchange and correlation effects via various local-field correction functions suppresses the Fermi energy in comparison with the static H-screening effect. The maximum influence of local-field correction is observed due to T-screening function and minimum influence is observed for H-function while most of the local field correction functions are found between them. As the direct comparison of the experimental properties for the liquid alkalis are not available in the literature. But the present results are found in predictive nature. The

oscillatory behaviour seen in the Figures 1-5 indicate that the electron dispersion may have an important effect on the electronic properties of liquid metals.

4.   Conclusions

From the present study we conclude that, among all the liquid alkalis, it was observed that liquid Cs has largest negative hump in the electron dispersion among all the alkalis. The depth of the negative hump in the electron dispersion of liquid alkalis increases in the order Li→Cs, while the magnitude of the first positive peak decreases. Among all the liquid alkalis, minimum deviation in the Fermi energy at Fermi level is obtained for 'Li' and the maximum for 'Cs'. Our model potential with more advanced IU, F and S-local field correction functions generate consistent results regarding the electronic properties of liquid alkalis and found suitable. Also, the present investigation predicts that the electronic properties of liquid alkalis are sensitive to the selection of the proper local field correction function. Such study will also be extended for another liquid metals and their alloys and communicated in future.

References

[1]   Y. Waseda, Structure of Non-Crystalline Materials, McGraw-Hill Pub. Co., New York (1980).
[2]   A. M. Vora, J. Adv. Phys. 4 (2015) 164.
[3]   Aditya M. Vora, Inter. Lett. Chem., Phys. Astro. 54 (2015) 56.
[4]   Aditya M. Vora, Phys. Chem. Liq. 49 (2011) 493.
[4]   Aditya M. Vora, Phys. Chem. Liq. 4 (2009) 663.
[5]   Aditya M. Vora, Commun. Theor. Phys.54 (2010) 159.
[6]   S. K. Srivastava, J. Phys. Chem. Solids 36 (1975) 993.
[7]   S. K. Srivastava and R. Dawar, Indian J. Pure Appl. Phys. 31 (1993) 520.
[8]   P. N. Gajjar, B.Y. Thakore and A. R. Jani, Acta Phys. Polo. A94 (1998) 33.
[9]   M. H. Patel, A. M. Vora, P. N. Gajjar and A. R. Jani, Physica B304 (2001) 152.
[10]   M. H. Patel, A. M. Vora, P. N. Gajjar and A. R. Jani, Commun. Theor. Phys. 38 (2002) 365.
[11]   J. K. Percus and G. J. Yevick, Phys. Rev. 110 (1958) 1.
[12]   W. A. Harrison, Elementary Electronic Structure, World Scientific, Singapore (1999).
[13]   R. Taylor, J. Phys. F: Metal Phys. 8 (1978) 1699.
[14]   S. Ichimaru and K. Utsumi, Phys. Rev. B24 (1981) 7385.
[15]   B. Farid, V. Heine, G. E. Engel and I. J. Robertson, Phys. Rev. B48 (1993) 11602.
[16]   A. Sarkar, D. S. Sen, S. Haldar and D. Roy, Mod. Phys. Lett. B12 (1998) 639.

Table 1   Input parameters and other constants.

Alkalis	Z	Ω_O (au)^3	σ (au)	η	r_C (au)
Li	1	146.46	5.0484	0.46	1.6677
Na	1	266.08	6.1601	0.46	2.0349
K	1	480.84	7.5033	0.46	2.4786
Rb	1	627.15	8.0158	0.43	2.7081
Cs	1	775.73	8.6045	0.43	2.9070

Table 2   Fermi energy $-E_F$ (10^{-12} erg) for liquid alkali metals.

Metals	Present results					Others [4-8]
	H	T	IU	F	S	
Li	6.9175	6.7740	6.8846	6.8079	6.8549	6.8584, 6.9480, 6.9623, 6.9855, 7.0021, 7.0443, 7.0633, 7.0662, 7.0679, 7.0805, 7.0861, 7.0961, 7.1023, 7.1149, 7.1468, 7.2530, 7.2965, 7.3989, 7.4199
Na	4.4983	4.3345	4.4619	4.3813	4.4303	4.6934, 4.7008, 4.7057, 4.7199, 4.7388, 4.9170, 4.9283, 4.9406, 4.9544, 4.9578, 4.9596, 4.9709, 4.9724, 4.9755, 4.9856, 5.0477, 5.0566, 5.0879, 5.0986
K	2.8920	2.7006	2.8512	2.7640	2.8174	3.1559, 3.1701, 3.2081, 3.2184, 3.2811, 3.2922, 3.3030, 3.3105, 3.3270, 3.3306, 3.3328, 3.3404, 3.3448, 3.3493, 3.3610, 3.3663, 3.3664, 3.3688, 3.3725
Rb	2.3315	2.1147	2.2864	2.1865	2.2475	2.5617, 2.6042, 2.6250, 2.6503, 2.6752, 2.7025, 2.7448, 2.7620, 2.7697, 2.7703, 2.7755, 2.7668, 2.7699, 2.7802, 2.7919, 2.8390, 2.8662, 2.8755, 2.9007
Cs	1.9685	1.7378	1.9216	1.8180	1.8817	2.1582, 2.1592, 2.1783, 2.1800, 2.1977, 2.2119, 2.2262, 2.2436, 2.2744, 2.3012, 2.3292, 2.3293, 2.3354, 2.3488, 2.3559, 2.4294, 2.4396, 2.4617, 2.4724

Guide to the Figures

Fig. 1. Electron dispersion curves for liquid Li.
Fig. 2. Electron dispersion curves for liquid Na.
Fig. 3. Electron dispersion curves for liquid K.
Fig. 4. Electron dispersion curves for liquid Rb.
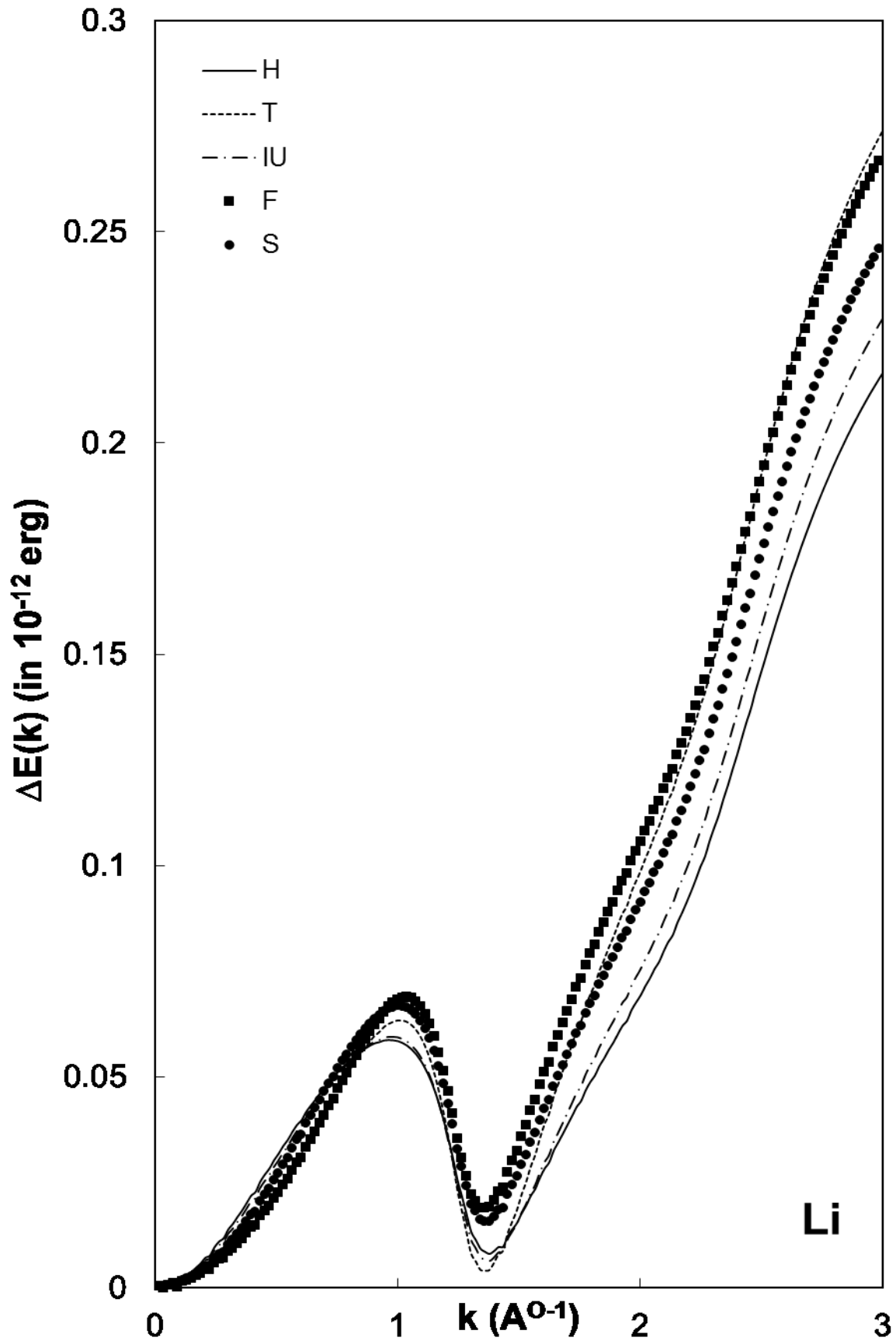Fig. 5. Electron dispersion curves for liquid Cs.

Fig. 1

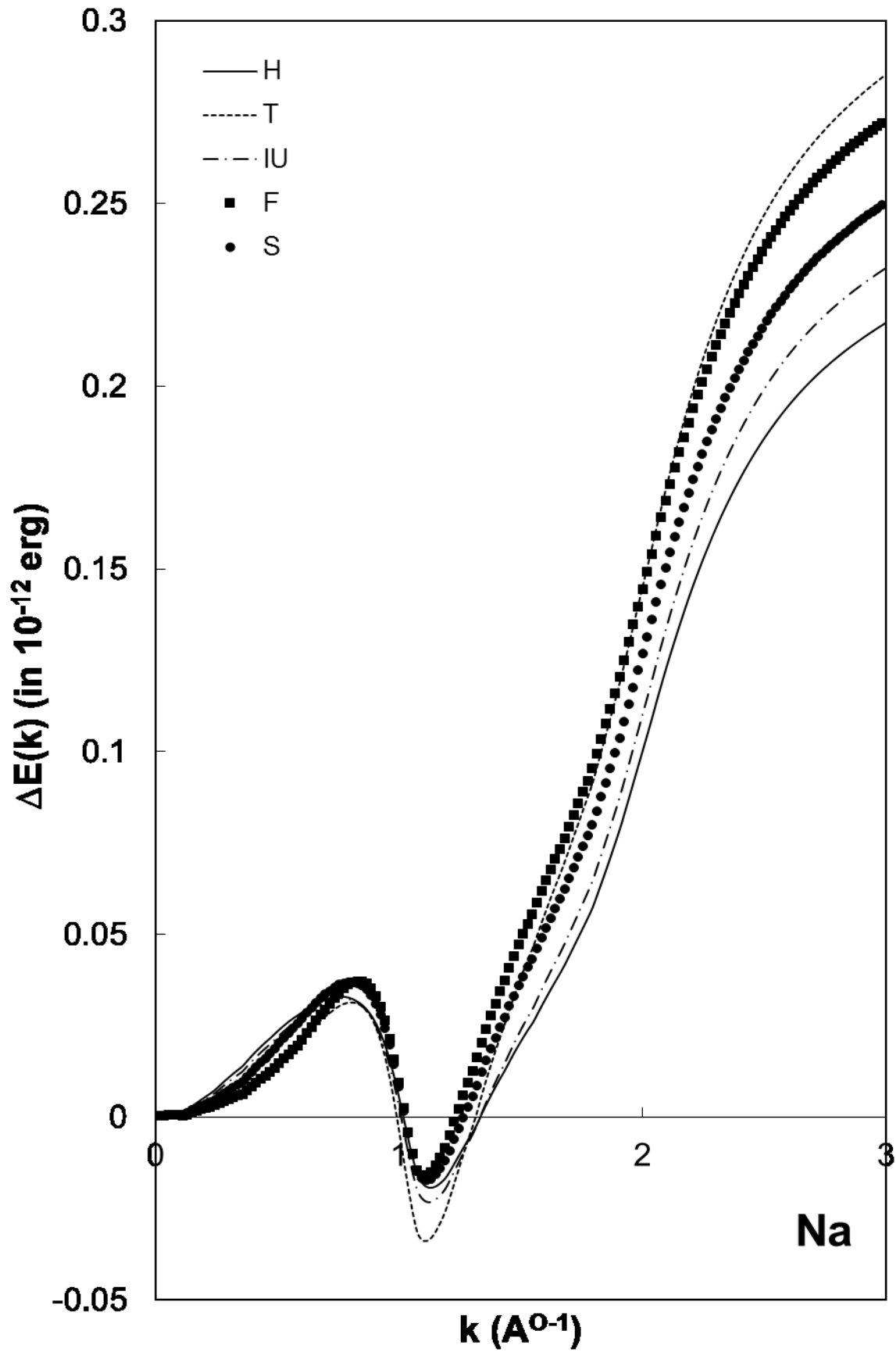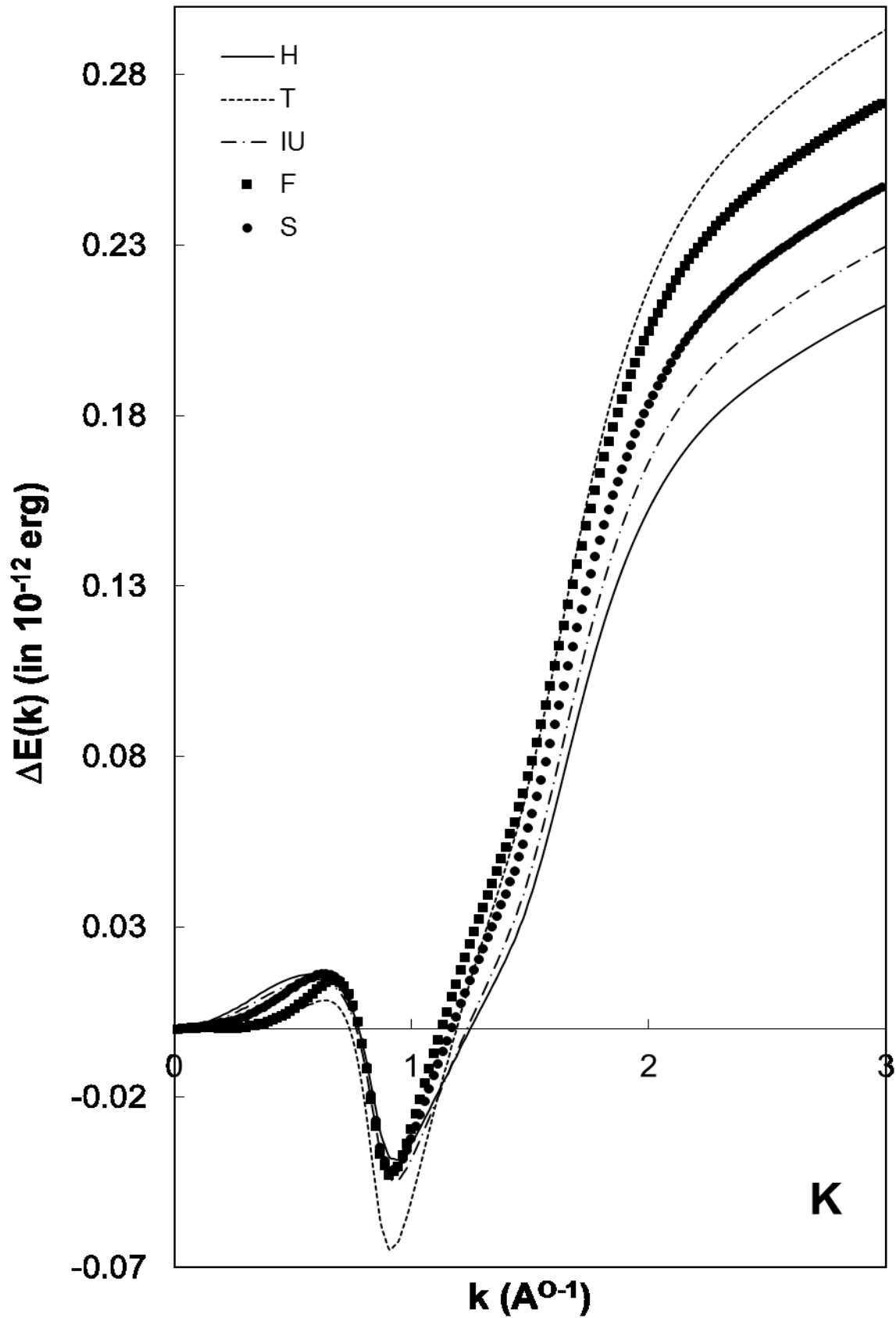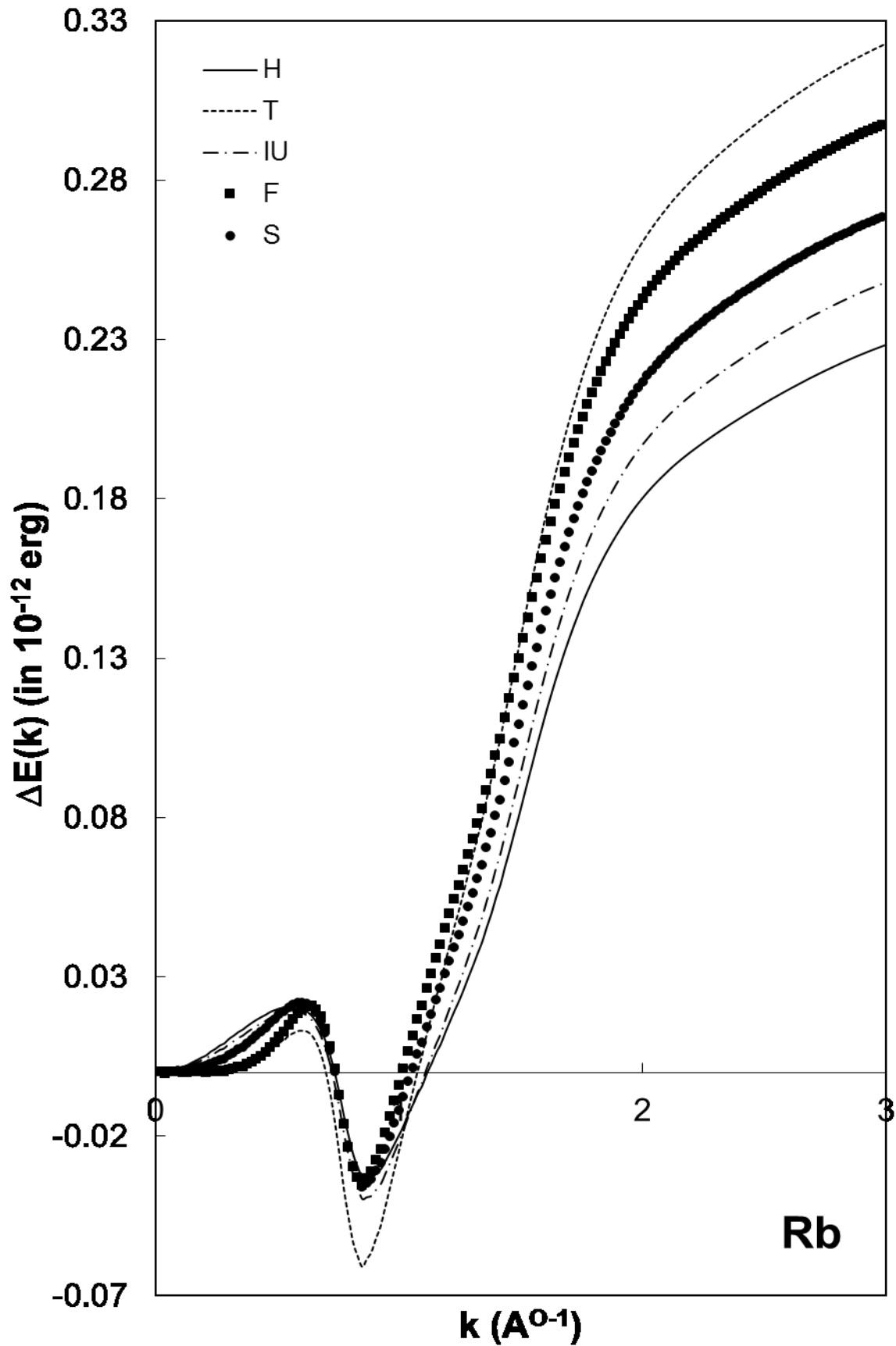Fig. 2

Fig. 3

Fig. 4

Fig. 5