Abstract Submitted for the MAR07 Meeting of The American Physical Society

Possible Mechanism of the Pseudogap Formation in Intermetallic Compound  $Al_3V$  SUSUMU MIYAHARA, KAZUO TSUMURAYA, Meiji University, JAPAN — The pseudogaps in compounds give a unique electronic character in the materials such as the ones in the skutterudites. The  $Al_3V$  compound with DO<sub>22</sub> structure has also a deep pseudogap that has been explained by the presence of the covalent Al-V and Al- Al bonds in the compound [1]. We propose another possibility of the formation of the pseudogap in the DO<sub>22</sub> compound using a density functional method. We introduce a Peierls distortions along c-axis of the double-stacked ordered unit cell, we calculate the density of states and check the gap formation. We will apply the mechanism to the other systems with pseudogap. [1] M. Krajčí and J. Hafner, J. Phys.: Condens. Matter, 14, 1865 (2002).

> Susumu Miyahara Meiji University, JAPAN

Date submitted: 20 Nov 2006

Electronic form version 1.4