**First Principle Study of Non-thermal Phase Transition Mechanism with Uniaxial Stress Applied Phase Transition Material : GeTe**

Hanjin Park,1 Won Jun Yang2, Dasol Kim2, Seung Jong Park2, Mann-Ho Cho2,\*, and Young-Kyun Kwon1,\*

*1Department of Physics and Research Institute for Basic Sciences, Kyung Hee University, Seoul, 130-701, Republic of Korea*

*2Institute of Physics and Applied Physics, Yonsei University, Seoul 120-749, Republic of Korea*

1, \* E-mail: [ykkwon@khu.ac.kr](mailto:ykkwon@khu.ac.kr)

2, \* E-mail: mh.cho@yonsei.ac.kr

Recently, phase change materials (PCM) have attracted attention as candidate for next generation memory device elements. But it has several problems in power consumption, information storage capacity, energy efficiency, and so on. We use *ab initio* density functional theory to investigate *non thermal* phase transition of a prototypical phase change material, GeTe, induced by uniaxial strain. We focus on the rhombohedral structure which can be interpreted as a layered strucuture, in which layers are seperated by long bonds. It is found that GeTe layered structure experiences a phase transition from one crytalline phase to the other crystalline one under external uniaxial tensile stress. We identify that the latter phase is essentially regarded as another layered structure rotated from the former phase through the exchange mechansm between short and long bonds. Our electronic transport calculation also shows that the conductance changes significantly during such phase transition, implying that uniaxial strain may induce non-thermal phase transition in GeTe.