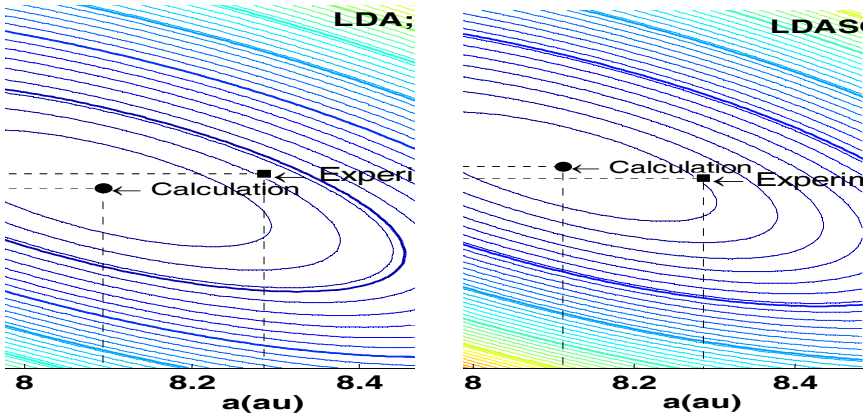
Spin Orbit Coupling and Correlation Effect on the Structural Optimization of Telluride Alloys ; First-principles Approach

Tran Van Quang[1*] and Miyoung Kim[2]
[1]Dept of Physics Hanoi Univeristy of Transport and Communications, Vietnam
[2]Dept of Nano Physics, Sookmyung Women's University, Korea

Correlation effect due to the strongly localized electronic bands often needs to be treated with additional terms beyond the general exchange correlation potentials such as the local density approximation (LDA). Spin-orbit coupling also plays crucial role for most of materials in this category. Here, we report the first-principles investigation on the effect of the correlation and spin-orbit coupling interactions on the structural optimization for telluride alloys. The all-electron full-potential linearized augmented plane-wave (FLAPW) [1] method is employed within LDA with and without +U and the second variational treatment of spin-orbit coupling is adopted. We found that the optimized lattice constants of the telluride alloy are affected by SOC as shown in the figures below and the lattice distortion upon the Gd doping is critical to precisely determine the conducting property.



참고문헌

[1] E. Wimmer, K. Krakauer, M. Wienert, and A.J. Freeman, Phys.Rev B **24**, 864 (1981).