Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Finding the structure of phosphorus in phase IV by the first-principles calculation TAKAHIRO ISHIKAWA, HITOSE NAGARA, KOICHI KUSAKABE, NAOSHI SUZUKI, Osaka University — Phosphorus in phase IV (P-IV) had been unclear since first experimental report. Using the metadynamics combined with the first-principles calculation, we obtained a new structure. The structure is a monoclinic of sc: a=c=4.22Å, b=4.15Å, β=97.76° and a modulation is observed along the b-axis. We noted this modulated pattern and, for modulated structures having other wave-lengths, compared the x-ray diffraction patterns of these structures with experimental one. As a result, limited to the case of commensurate patterns because of the periodic boundary condition for the calculations, the structure whose period is 4 times as long as that of the non-modulated structure is the most compatible for the experimental result. For this pattern, calculating the enthalpy for pressure, it is lower than both sc and sh in the range from 118 GPa to 128 GPa. Recently Akahama *et al.* have determined the structure of P-IV, which is rather close to our structure. Our calculation shows the transition from sc to P-IV was the first order phase transition.

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Date submitted: 03 Dec 2005 Electronic form version 1.4