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First-principles study of the noncentrosymmetric superconductors Li_2Pt_3B and Li_2Pd_3B TATSUYA SHISHIDOU, ADSM, Hiroshima Univ, TAMIO OGUCHI, ISIR, Osaka Univ — Effect of spin-orbit coupling (SOC) associated with lack of space-inversion symmetry has been a central issue in condensed-matter physics. Li_2Pt_3B and Li_2Pd_3B are superconducting below 2.7 K and 7 K, respectively, and have the same crystal structure (cubic $P4_332$, No. 212), which is noncentrosymmetric and is characterized by highly distorted corner-sharing $BPt(Pd)_6$ octahedra. Despite the same valency and structure, they show quite different superconducting behavior. NMR measurements [1] indicate that Li_2Pt_3B would be a spin-triplet superconductor with line nodes in the gap function while Li_2Pd_3B is a conventional spin-singlet s-wave superconductor. SOC would be a key to understand this difference. To clarify the electronic band structure and Fermi surface of these compounds, we performed density-functional (GGA PBE) calculations with FLAPW method. Relativistic effects were fully taken into account. The band structures calculated are in good accordance with previous work[2] and the spin splitting due to SOC is quite significant in Li_2Pt_3B. This work was supported by a MEXT KAKENHI on Innovative Areas "Topological Quantum Phenomen". [1] M. Nishiyama, Y. Inada, and G.-q. Zheng, PRL **98**, 047002 (2007); PRB **71**, 220505(R) (2005). [2] K.-W. Lee and W. E. Pickett, PRB **72**, 174505 (2005).

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