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Quantized Zak Phase and Topological Surface Charge originating from the Nodal Line MOTOAKI HIRAYAMA, Dept. of Physics, Tokyo Tech.; TIES, Tokyo Tech., RYO OKUGAWA, Dept. of Physics, Tokyo Tech., SHUICHI MURAKAMI, Dept. of Physics, Tokyo Tech.; TIES, Tokyo Tech. — Recent study for the topological phenomena reveals that the singularity of the band structure in the k-space plays a significant role for both the bulk and surface properties. The semimetals having such a singularity include the Dirac semimetals, Weyl semimetals [1], and the nodal-line semimetals [2]. In this study, we focus on the nodal-line physics. One of the typical origin of the nodal-line is mirror symmetry, and the other is the π Berry phase. In the latter case, the Zak phase is either π or 0 depending on the momentum regions divided by the nodal lines, and the π Zak phase is related to bulk charge polarization, appearing as a surface polarization charge. We discuss the relation between the quantized Zak phase and the surface charge by using electronic calculations for the realistic materials such as fcc calcium and other systems. We also propose the concept of the π Zak phase is useful for novel behaviors of polarizations in insulators. [1] M. Hirayama, R. Okugawa, S. Ishibashi, S. Murakami, and T. Miyake, Phys. Rev. Lett. 114, 206401 (2015). [2] M. Hirayama, R. Okugawa, T. Miyake, and S. Murakami, arXiv:1602.06501 (Nat. Commun., Accepted).

Motoaki Hirayama
Dept. of Physics, Tokyo Tech.; TIES, Tokyo Tech.

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