Walther-Meißner-Seminar

Walther-Meißner-Institute, Seminar Room 143

Date: **Friday, 25 October 2024, 11:15 h**

Speaker: **Dr. Takahiko Sekine**

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Title: **Site-selective NMR investigation of local spin susceptibility in α-$(BETS)_2I_3$**

Abstract:
Dirac fermions are pseudo-relativistic massless quasiparticles in solids, which are expected to present exotic physical properties. α-D_2I_3 (D = BEDT-TTF, BETS) are candidates for a Dirac-fermion system with strong electron correlations. Due to the correlations, α-(BEDT- TTF)$_2I_3$ shows a charge-ordered insulator transition [1]. Although a selenium-analog α- $(BETS)_2I_3$ also shows a metal-insulator transition, recent X-ray diffraction experiments have demonstrated that an insulator state in α-$(BETS)_2I_3$ is not a charge-ordered state [2]. This finding indicates that an electronic state in α-$(BETS)_2I_3$ is distinct from that in α-(BEDE- TTF)$_2I_3$. An urgent task is to elucidate an electronic state in α-$(BETS)_2I_3$, which hosts the potential to discover novel physics in the Dirac fermion system.

We performed ^{13}C-NMR measurements using a single-crystal α-$(BETS)_2I_3$. The central double-bonded carbons on BETS molecules are enriched by ^{13}C isotopes. There are three independent molecular sites, A (= A′), B, and C, in the unit cell. The NMR spectra from the ^{13}C spins on every site did not show splitting on cooling down to 2 K, indicating the absence of a charge-ordered or a magnetic-order state as indicated in the previous study [3]. From the NMR spectral shifts, we successfully estimated local spin susceptibilities, χ^{μ}, on each site. The site dependence ($\chi^{C} > \chi^{A,A'} > \chi^{B}$) and the temperature dependence are similar to those in α-(BEDT-TTF)$_2I_3$ under high pressure with the Dirac-cone band [4]. This suggests that the characteristics of their bands are relatively common. Given that α-$(BETS)_2I_3$ exhibits insulating resistivity at low temperatures, a small band gap opens around Dirac points, which is likely provided by spin-orbit interactions enhanced by selenium substitution.

References
[1] M. Inokuchi et al., Bull. Chem. Soc. Jpn. **68**, 547 (1995).
[2] S. Kitou et al., PRB **103**, 035135 (2021).
[3] T. Konoike et al., JPSJ **91**, 043703 (2022).
[4] M. Hirata et al., Nat. Commun. **7**, 12666 (2016).

gez:
Mark Kartsovnik (Host)