Fundamental Quantum Science Program
Seminar series No.2

●Date & Time : **Monday 20th May 2024 10:30-12:00**
●Venue : #154 156, Main Research building

Prof. Noejung Park

Ulsan National Institute of Science and Technology (UNIST), Department of Physics

" Real-time time-dependent density functional theory calculations of spin-orbit dynamics and Berry-curvature characteristics of solid states"

We have used the real-time time-dependent Kohn-Sham equations, within adiabatic local density approximation, to reveal various Berry-curvature characteristics of solid states. We successfully demonstrated that the quantum anomalous Hall conductivity and the quantum spin Hall conductivity of real-material bulk topological insulators can be directly obtained in the real-time profile. We now extend our study to nonlinear optical responses associated with spin-orbit dynamics. We particularly focus on the situation when a built-in geometrical chirality is exposed to an axial electric field and/or magnetic field, or even non-zero $\boldsymbol{E} \cdot \boldsymbol{B}$. We discuss that the consequent charge-orbit dynamics can be compared with the Thouless charge pump model, and also be partly analogous to the axial anomaly of gauge field theory. We discuss the limitation and utility of local spin density approximation for the exchange-correlation magnetic field in the aforementioned spin-orbit dynamics.

・Hosted by : Dr. Naoto Nagaosa
(Fundamental Quantum Science Program)