# Time-dependent density functional theory calculations for spin-phonon-polarization dynamics and band topology

Mahmut Sait Okyay, Beomseop Kim, Noejung Park

*Department of Physics, UNIST, UNIST-gil 50, Ulsan 44919, Republic of Korea*
*noejung@unist.ac.kr*

Topological characterization has now been a key ingredient of present materials study, and global properties immune to local perturbations have been suggested in terms of topological invariants. Topological numbers of real materials have been evaluated through the theories of linear responses over the static ground electronic structure [Kubo formula]. Here, we present that the real-time dynamics can be alternatively used in the evaluation of topological state. By tracing the real-time evolution of the system, incurred by a time-evolving parameter of Hamiltonian, we can obtain the Berry phase accumulated over the time-evolving wave function. As an example, we deal with a trivial insulator, a spin-frozen valley-Hall system, a spin-frozen Haldane-Chern insulator, and a quantum spin-Hall insulator. [1] We also demonstrate that the TDDFT-based real-time dynamics can be an efficient tool for nonlinear dynamics of strongly coupled system. We present the spin dynamics of $MoS_2$ induced by a pumped phonon through strong spin-orbit coupling. [2] High harmonic responses and nonlinear Hall current under a high intensity light field will be demonstrated. [3] Specifically, we focus on the second-order nonlinear Hall current which can be thought of a new method revealing the Berry curvature distribution.

[1] D. Shin et al., *PNAS*, **116** (10), 4135-4140 (2019)
[2] D. Shin et al., *Nat. Commun.*, **9**, 638 (2018)
[3] M. S. Okyay et al., *Phys. Rev. B* **102**, 104304 (2020)

ISBN 978-89-89453-30-7 