Riichiro Saito

M. Villa*, N. T. Hung, P. F. Rizky, M. S. Ukhtary, S. Roche*

Department of Physics, Tohoku University, 6-3 Aoba, Aramaki, Aoba-ku, Sendai, 980-8578, Japan
* Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Bellaterra, 08193 Barcelona, Spain

rsaito@flex.phys.tohoku.ac.jp

Tunable circular dichroism and valley polarization in two dimensional materials

In two-dimensional materials, it is known that there are several freedoms for the electronic states such as spin, pseudo-spin and valley-spin that can be observed near the K or K' valley in the hexagonal Brillouin zone. Although these freedoms are considered to be independent of one another, some of the freedoms appear at the same time and they can not be controlled to be independent by changing external parameters of the materials. For example, in the transition metal dichalcogenides, the valley polarization (VP) and pseudo-spin polarization (PP) occur simultaneously in which the VP can be explained by the pseudo-spin information of the wave function. Thus a fundamental question arises whether these freedoms are independent.

In order to estimate the question of two-dimensional physics, we adopt a general Hamiltonian so-called modified Haldane model that represents the hexagonal, two-dimensional materials including graphene, silicene, transition metal dichalcogenides, h-BN and so on. By solving the modified Haldane model, we show that the freedoms of PP and VP can be tuned independently as shown in Table I by selecting a proper set of the parameters of the Hamiltonian, which is a goal of the papepr. [1]
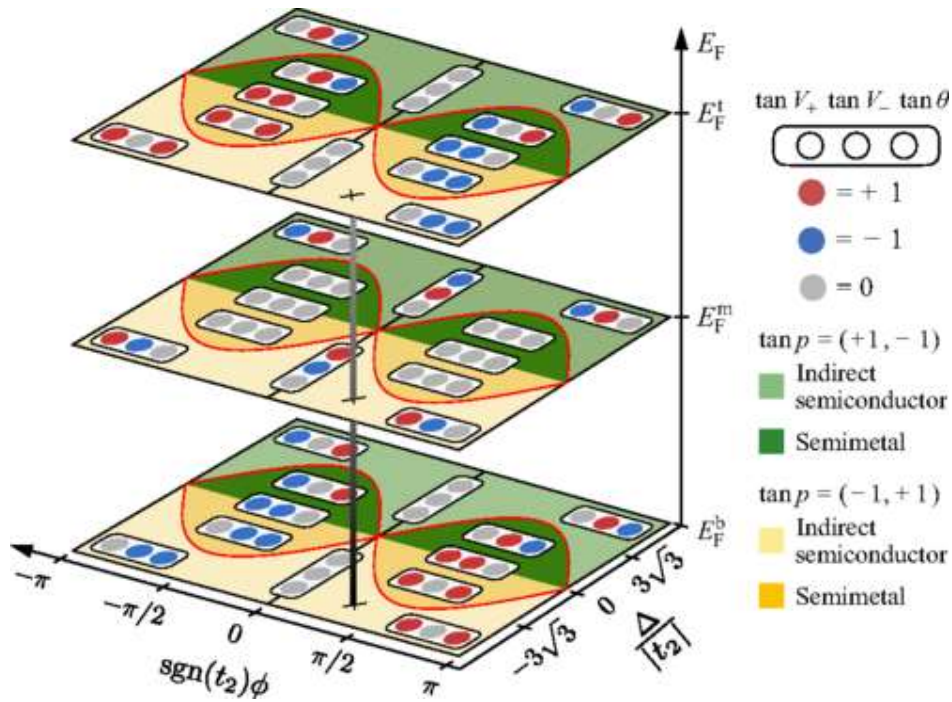

Figure 1: A phase diagram of the ground state of the modified Haldane model in which the ground states can be classified by valley polarization (tan V), pseudo-spin polarization (tan p) and degree of circular dichroism (tan θ) as a function of the scaled parameters sign($(t_2)\phi$, $\Delta/|t_2|$, and the Fermi energy E_F. [1]

Tunable freedom can be observed in the optical measurement of circular dichroism (CD)of the material or resonant Raman spectroscopy. Circular dichroism is defined by the difference of absorption probabilities of the material for left-handed and right-handed circularly polarized lights. In the Raman spectroscopy, the helicity conserved (or changing) Raman process can be observed for understanding the valley polarization. In particular, the conservation rule of angular momentum of a phonon in the Raman spectroscopy is discussed for a given phonon mode in the connection of the present problem. [2]

In the early works, we found by solving the (not modified) Haldane model in which perfect circular dichroism appears in a particular case of the parameters of the Haldane model in which time-reversal symmetry is broken by the so-called $\varphi \neq 0$ parameter. [3] However, within the Haldane model, the freedoms of VP, that can be expressed by a dimensionless relative intensity of optical absorption, tan V, and the freedom of PP, tan p can not be independent. [3] When we further consider the breaking symmetry of valley freedom by introducing the parameter $\Delta \neq 0$ in the modified Haldane models, we can get the results in which valley polarization (tan V), pseudo-spin polarization (tan p) and degree of circular dichroism ($\tan \theta$) can change independently as a function of the scaled parameters $\text{sign}((t_2)\phi$, $\Delta/|t_2|$, and the Fermi energy E_F as shown in the phase diagram (Fig. 1). This results can be compared with the existing materials and predicting some new two-dimensional materials which shows a perfect circular dichroism or pseudo-spin polarized states as a function of laser excitation energy. [4] We will discuss the present theoretical models with some new materials that are observed in the experiment.

References

[1] M. Villa, N. T. Hung, S. Roche, R. Saito, Phys. Rev. B, 99 (2019) 161404.
[2] Y. Tatsumi, T. Kaneko, R. Saito, Phys. Rev. B, 97, (2018) 195444.
[3] K. Ghalamkari, Y. Tatsumi, R. Saito, J. Phys. Soc. Jpn., 87 (2018) 063708.
[4] P. F. Rizky, M. S. Ukhtayry, R. Saito in preparation.

TABLE I. Combinations of the presence (◯) and absence (X) of pseudospin, valley polarization, and circular dichroism, and the materials/models where such combinations occur. The Haldane/modified Haldane model is abbreviated as H/mH. [1]

PP	VP	CD	Model/Material
X	X	X	Graphene, H and mH[a]
X	X	◯	
X	◯	X	H,[b] mH[c]
X	◯	◯	
◯	X	X	mH[d]
◯	X	◯	H[e]
◯	◯	X	hBN, TMD, H,[f] mH[g]
◯	◯	◯	mH[h]

[a] $\Delta=\varphi=0$, E_{mF} (semimetal, $\Delta=0$).

[b] $\Delta/t_2=3\sqrt{3}$.

[c] $E_{b,tF}$ ($\Delta=0$).

[d] E_{mF} (semimetal, $\Delta\neq0$), $E_{b,tF}$ ($\varphi=0$).

[e] Topological insulator.

[f] Trivial insulator.

[g] E_{mF} (indirect semiconductor).

[h] $E_{b,tF}$ ($\Delta\neq0$, $\varphi\neq0$).