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Theoretical Study on Circularly Polarized Light Absorption in Triptycene Molecular Membrane

We numerically analyze the light absorption intensity of triptycene molecular membrane (TMM) under the circularly-polarized light irradiation. Since the lattice structure of TMM provides the Kagome-lattice-like network for its π-electrons, the electronic structures of TMM should have the characteristic energy band structures of Kagome lattice, i.e. π-electronic band structure of graphene with a flat band. Recent first-principles calculations using density functional theory (DFT) confirmed the existence of Kagome-like energy band structures in TMM [1]. Owing to the presence of flat band, it is also expected to have characteristic optical properties in this system. In this paper, we build the tight binding model which reproduce the energy band structures obtained from DFT, and evaluate the light absorption intensity under the circularly-polarized light irradiation using Kubo formula.

Figure 1 (a) shows the schematic lattice structure of TMM. The energy bands spectrum and density of states of TMM are shown in Fig.1 (b), where several Kagome-like bands, i.e. graphene band and flat bands, are observed. The graphene bands have the valley structures around K and K' points. Since the space inversion symmetry is broken in TMM, the circularly polarized irradiation can selectively excite the electrons either K or K' point, resulting in the appearance of valley polarization.

Figure 1 (c) shows absorption intensities in momentum space for the inter-band transition between the graphene bands, where no clear valley-dependent excitation is not observed. However, as shown Figure 1 (d), the inter-band transition from the graphene-like band to the flat band clearly show the valley-selective optical excitations by circularly polarized light irradiation. Thus, our numerical analysis shows that TMM can be a good candidate material for the application to valleytronics.

References

[1] Y. Fujii, M. Maruyama, K. Wakabayashi, K. Nakada, and S. Okada. J. Phys. Soc. Jpn. 87, 034704, (2018).

Figures

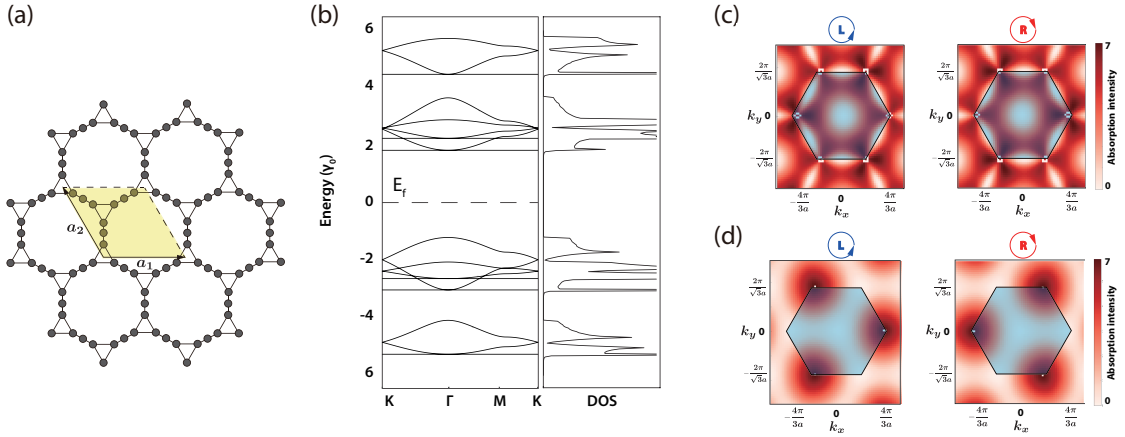

Figure 1 (a) Lattice structure of TMM. (b) Energy band structure of TMM. The electronic structure of TMM is a direct semiconductor material composed of multiple Kagome-like bands. (c) Intensity of light absorption in momentum space for the optical inter-band transition between the graphene-like bands. (d) Same for transition flat band to graphene band.