Max-Planck-Institut für Struktur und Dynamik der Materie



Max Planck Institute for the Structure and Dynamics of Matter

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Optical Materials Design of Transition-Metal Dichalcogenides and Frustrated Mott Insulators

Spurred by recent progress in melting, enhancement and induction of electronic order out of equilibrium, a tantalizing prospect concerns instead accessing transient Floquet steady states via broad pump pulses, to affect electronic properties. Here, we discuss a two-pronged approach to manipulate the topology of a band insulator, as well as topological order in a Mott insulator. We first consider monolayer transition-metal dichalcogenides (TMDCs), and show that their low-energy description as massive 2D relativistic fermions fails to hold for optical pumping. Instead, the added complexity of a realistic materials description leads to a novel mechanism to optically induce topologically-protected chiral edge modes, facilitating opticallyswitchable conduction channels that are insensitive to disorder. We develop a strategy to understand non-equilibrium Floquet-Bloch bands and topological transitions directly from ab initio calculations, and illustrate for the example of WS2 that control of chiral edge modes can be dictated solely from symmetry principles and is not qualitatively sensitive to microscopic materials details. Second, we extend these ideas to strongly-correlated systems and show that pumping frustrated Mott insulators with circularly-polarized light can drive the effective spin system across a phase transition to a chiral spin liquid (CSL). We find that the transient time evolution of a Kagome lattice Hubbard model is well-captured by an effective spin description, where circular polarization promotes a staggered scalar spin chirality Si (Si × Sk) directly to the Hamiltonian level. We fingerprint the ensuing phase diagram and find a stable photoinduced CSL in proximity to the equilibrium ground state. The results presented suggest new avenues to marry dynamical symmetry breaking, strong interactions, and ab initio materials modelling, to access elusive phase transitions that are not readily accessible in equilibrium.



