Organic Dirac Materials

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Dirac Materials is a prominent example of quantum materials where low energy particles obey the relativistic Dirac equation in contrast to conventional Schrodinger equation. I will present recent theory work on Dirac materials covering two aspects:

i) extension of Dirac materials to include materials with boson excitations- so called Boson Dirac Materials that host boson exhibiting Dirac spectrum. Boson excitations on a non-Bravais lattices, like honeycomb lattice, will have multiple species that would induce the band crossing and Dirac nodes in the spectra, similar to graphene. An interesting and relevant example is the case of honeycomb ferromagnets with magnon Dirac nodes. We show how the Dirac spectrum leads to significant deviations in the magnon behaviour from the predictions of Dyson theory [1]. We were able to address long standing paradoxes in the observed spectra of Cr-trihalides like CrI3. [2] The predicted effects are especially relevant for the recently observed 2D honeycomb ferromagnets. [3]

ii) Rapid growth of computational power and high demand for prediction of materials with target properties have led to a new way of doing materials research referred to as materials informatics. This approach places the main effort on performing high-throughput computing combined with data mining. Applications of this data-driven approach are wide-ranging and cover the search for various quantum materials with special electrical, optical and magnetic properties. We have created the organics materials database (https://omdb.diracmaterials.org/) (OMDB) that hosts more electronic structures of more than 25000 compounds.[4] We used large scale search capability within OMDB to identify novel Dirac materials and materials with small gaps. Small gap semiconductors are said to be the key element for new detector materials for Dark Matter. We show how we can use large scale materials database to identify candidates for DM detection. [5]

References:

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