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Title of the Presentation: Topological Dirac nodal loops in nonsymmorphic hydrogenated monolayer boron

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Short Biography:

Research interests in science of monatomic layers and at surfaces, using advanced soft X-ray spectroscopies with high harmonic generation laser, X-ray free electron laser, and high-brilliant synchrotron radiation. Received many awards in surface science. The author/editor of the books, *2D Boron: Boraphene, Borophene, Boronene* (Springer, 2021) and *Monatomic Two-Dimensional Layers: Modern Experimental Approaches for Structure, Properties, and Industrial Use* (Elsevier, 2019).

Abstract:

Two-dimensional (2D) materials containing Dirac fermions have recently attracted intensive research attention for pursing fundamental science and developing quantum devices. Scientific and technological interests have maintained our efforts to synthesize new 2D materials and to discover novel electronic structures. Recently, fermions with Dirac nodal loops (DNLs) have been experimentally observed in several bulk materials. However, experimental observation of DNLs fermions in 2D materials is still lacking, excepting recent work on monolayers on metal substrates[1]. Free-standing 2D materials are much more convenient in experiments and in applications. The search for new and feasible synthetic free-standing 2D materials with DNLs fermions have attracted broad interests in condensed matter physics.

In this research, we predict the existence of DNLs in free-standing layers of hydrogenated monolayer boron sheets (borophane or HB) based on the topological band theory and first-principles calculations [2,3]. The DNLs are topologically protected by the local chemical bonding and non-symmorphic symmetry. The three-center two-electron bonds in the HB sheets restrict the electronic system to be semi-metallic with a nodal loop at the Fermi level or insulating. Two types of the electronic structures are distinguished by a Z_2 topological index. Moreover, the results are confirmed by band calculation of the density functional theory. The present topological classification can also be applied to the other atomic sheets to seek for novel Dirac Fermions.

[1] B. Feng, IM *et al*., Nature Comm., **8**, 1007 (2017).

[2] N.T. Cuong, IM *et al*., Phys. Rev. B **101**, 195412 (2020).

[3] I. Tateishi, IM *et al*., Phys. Rev. Materials **3**, 024004 (2019).