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M1Or1B-03: [Invited] Real-space screening of bulk topology of high-quality two-dimensional insulators

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Recent years have seen multiple high-throughput studies reveal an immense number of topological materials through use of symmetry indicators. Despite this success, three-dimensional topological insulators (TIs) admitting a band-gap larger than Bi₂Se₃ and two-dimensional TIs admitting a band gap larger than β -bismuthene, two of the originally proposed TIs, remain extremely rare, creating a bottleneck for progress in experiments and quantum devices. Simultaneously, a significant effort has been made to understand and identify topological phases “invisible” to symmetry indicators. Such phases offer a unique opportunity to expand the search for a large band-gap TI, however their identification requires sophisticated probes of bulk topology. Magnetic flux tubes or vortices have emerged as one such probe in two-dimensions when inserted into the bulk. In this work, we develop an automated workflow to perform vortex insertion and apply it to a current database of high-quality, experimentally realized, two-dimensional insulators. The results reveal multiple novel two-dimensional topological insulators supporting large bands gaps, including the 1H-MX₂ (M=Mo,W) and (X=S,Se,Te) family of transition metal dichalcogenides. Our work has broad implications for current theoretical and experimental efforts to employ these materials in superconducting and Moire systems.

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