PÔSTER - RESUMO - MATERIAIS E BIOMATERIAIS

UNRAVELING MN INTERCALATION AND DIFFUSION IN NBSE2 BILAYERS THROUGH DFTB SIMULATIONS

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The groundbreaking discovery of graphene in 2004 opened up a new era in two-dimensional (2D) materials, unveiling a rich spectrum of novel properties. Recently, a new method for synthesizing van der Waals heterolayers was introduced by reacting Bi2Se3 with transition metals, such as Mn or Cr, yielding XBi2Se4 (with X = Mn or Cr) layers on a Bi2Se3 substrate. The insertion of metal layers between TMDs enables the formation of new pseudo-2D materials that can exhibit a range of intriguing effects, including the quantum anomalous Hall (QAH) effect, quantized magnetoelectric response, and Majorana fermions [1]. Here, our study focuses on investigating the atomic-scale mechanisms of Mn intercalation and diffusion in NbSe2 bilayers through density functional tight-binding (DFTB) simulations [2]. Our work is directly motivated by recent experimental reports on Mn intercalation in NbSe2 [3], and we provide a theoretical view that helps interpret these findings. Our results present the energetics, diffusion pathways, and concentration-dependent behavior of Mn

atoms, offering a detailed understanding of the intercalation process and its influence on the material's properties.

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Palavras-chave: dftb; molecular dynamics; tmds; 2d materials.