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Stacking and Registry Effects in Layered Materials: The Case of Hexagonal Boron Nitride LEEOR KRONIK, NOA MAROM, Weizmann Institute of Science, JONATHAN BERNSTEIN, Tel Aviv University, JONATHAN GAREL, Weizmann Institute of Science, ALEXANDRE TKATCHENKO, Fritz Haber Institut, ERNESTO JOSELEVICH, Weizmann Institute of Science, ODED HOD, Tel Aviv University — The interlayer sliding energy landscape of hexagonal boron nitride (h-BN) is investigated via a van der Waals corrected density functional theory approach. It is found that the main role of the van der Waals forces is to anchor the layers at a fixed distance, whereas the electrostatic forces dictate the optimal stacking mode and the interlayer sliding energy. A nearly free-sliding path is identified, along which band gap modulations of 0.6 eV are obtained. We propose a simple geometric model that quantifies the registry matching between the layers and captures the essence of the corrugated h-BN interlayer energy landscape. The simplicity of this phenomenological model opens the way to the modeling of complex layered structures, such as carbon and boron nitride nanotubes. Reference: Marom et al., Phys. Rev. Lett. 105, 046801 (2010).

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