High-throughput design of high-performance high-k dielectrics for 2D electronics

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Two-dimensional (2D) semiconductors such as monolayer MoS_2 hold significant promise for advancing nanoelectronics. However, integrating high-k dielectrics with 2D semiconductors to achieve high performance remains a challenge. In this talk, I will present our understanding of designing high-performance interfaces between high-k dielectrics and 2D MoS_2. First, we demonstrate that hydrogenation is an effective method for passivating dangling bonds at the interface between conventional high-k dielectrics and MoS_2, in which hydrogenation selectively occurs on high-k dielectrics such as Si_3N_4 and HfO_2 without affecting the MoS_2. Second, we introduce a data-driven approach to expedite the discovery of promising inorganic molecular crystals as high-performance high-k dielectrics for 2D MoS_2. These findings advance the understanding of integrating high-k dielectrics with 2D semiconductors and could be useful for the development of a wide range of 2D electronic and optoelectronic devices.