Fluorinating Hexagonal Boron Nitride into Diamond-like Nanofilms with Tunable Band Gap and Ferromagnetism

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Outline:

1) Energetics comparison,

2) Molecular dynamics simulation.

3) Band structures of HF-BN nanofilms.

1) Energetics comparison

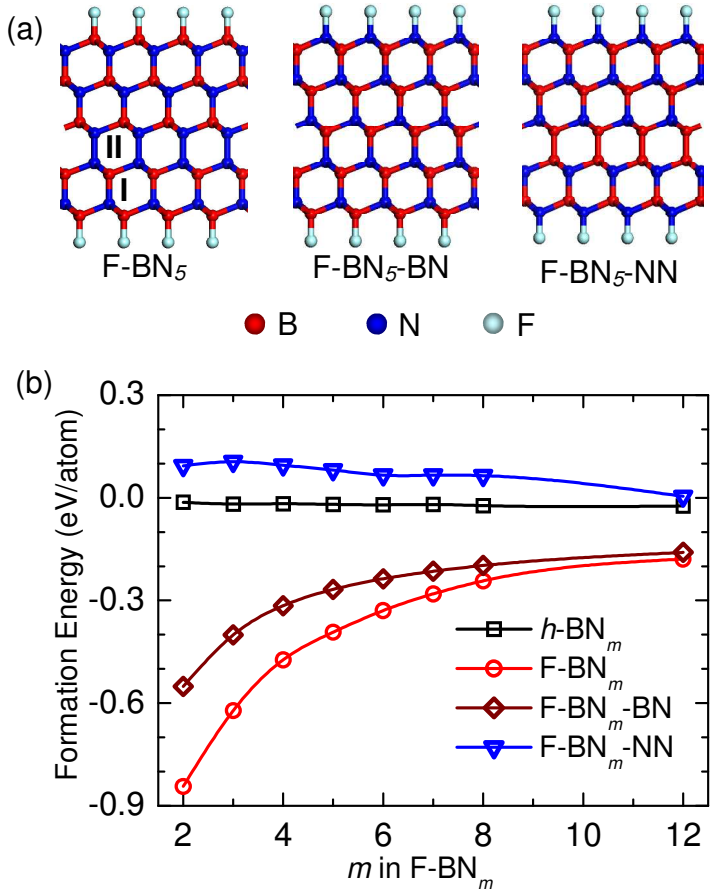

Figure S1. (a) Front views of atomic structures for the sp^3 bonded F-BN_m nanofilms with different termination atoms. (b) Formation energies of *h*-BN_m, F-BN_m, F-BN_m-BN and F-BN_m-BB nanofilms as a function of *m*. In the formed nanofilm, the N-N bond length is 1.48 Å in average, shorter than 1.59 Å of other B-N bonds.

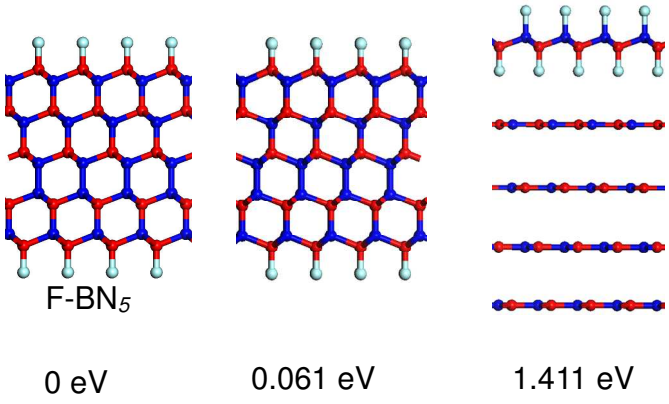

Figure S2. Front views of atomic structures for two possible polymorphs of the F-BN_5 nanofilms and their relative energies per unit cell with respect to the F-BN_5 nanofilms.

2) Molecular dynamics simulation

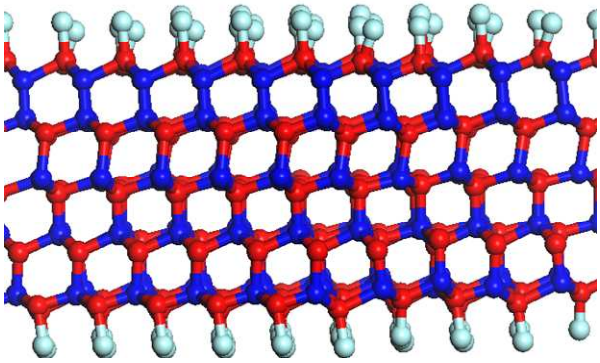

Figure S3. Snapshots of the F-BN_5 nanofilm at the end of 5ps quantum molecular dynamics simulations.

3) Band structures of HF-BN nanofilms.

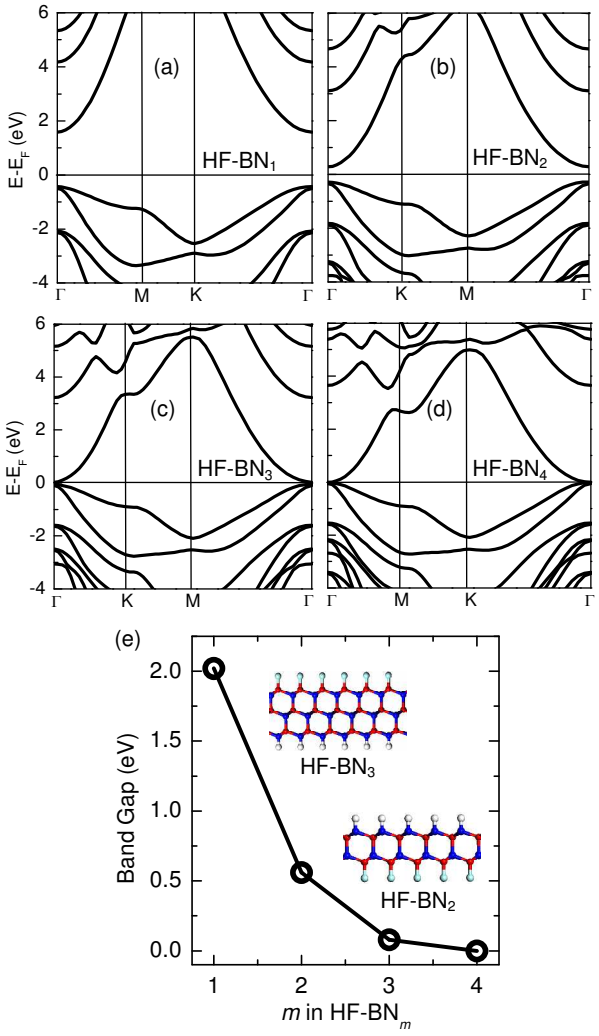

Figure S4. (a-d) Band structures of the HF-BN_m nanofilms. (e) Band gap as a function of m in the HF-BN_m nanofilm. Insets show the atomic structures of the HF-BN_3 and HF-BN_2 nanofilms.

A merit of these single-crystalline HF-BN nanofilms is their desirable electronic properties. For example, the HF-BN_3 nanofilm possesses a direct LDA gap of 0.08 eV and an effective electron mass of 0.95 m_0 (m_0 is the mass of free electron), close to that of silicon. Moreover, the LDA gap of the HF-BN nanofilms is reduced quickly with increasing film thickness and their structures are robust to carrier doping.