

Regulation of the Valleytronic Properties in Single-Layer NbSeCl

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Table SI The calculated relative energies (meV) of the NbSeCl/HfN₂ heterostructures (b), (c), (d), (e), (f) and (g) with respect to that of the configuration (a).

| configuration | (a) | (b) | (c) | (d) | (e) | (f) |
|---------------|-----|-----|------|-----|------|-----|
| ΔE | 0 | 3.2 | 45.6 | 7.7 | 43.5 | 4.0 |

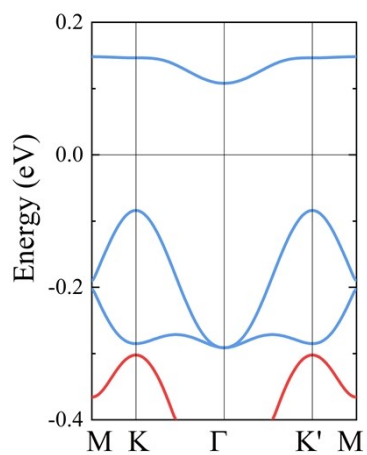


Fig. S1 The band structures of Cr-doped NbSeCl without SOC effect.

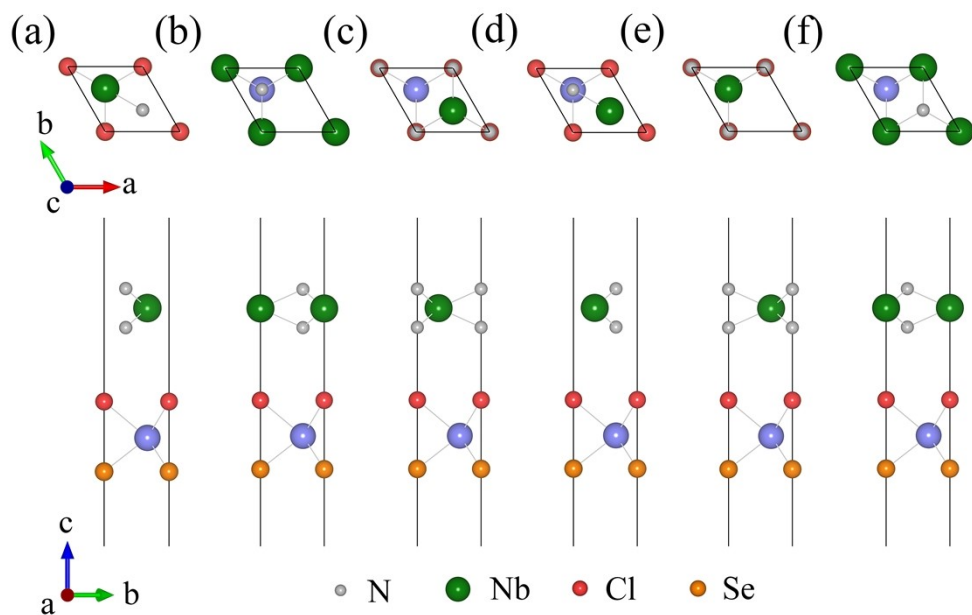


Fig. S2 (a) to (f) are top and side views of six NbSeCl/HfN₂ heterostructures. The blue, orange, red, green and gray balls represent Nb, Se, Cl, Hf and N atoms, respectively.

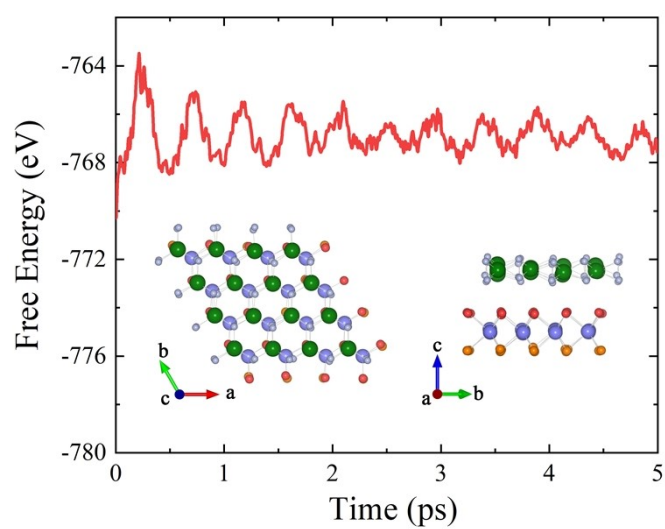


Fig. S3 Time evolution of free energy for NbSeCl/HfN₂ heterostructures at 300 K in AIMD simulation. The insets show the snapshot of atomic structure at 5 ps.

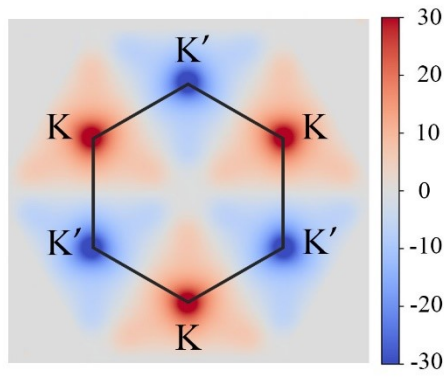


Fig. S4 Contour map of Berry curvature of NbSeCl/HfN₂ heterostructures over the entire 2D BZ.