iScience, Volume *27*

Supplemental information

Villin headpiece unfolding upon binding to boridene mediated by the “anchoring-perturbation” mechanism

Yuqi Luo, Zonglin Gu, Weihua Liao, Yiwen Huang, Jose Manuel Perez-Aguilar, Yanbo Luo, and Longzhen Chen

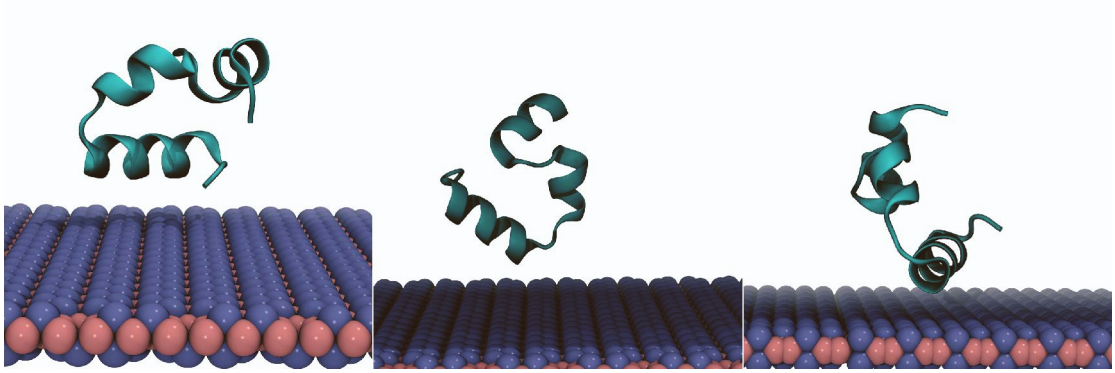

Figure S1. The final conformations of HP35 binding to boridene nanosheet at 2000 ns in three parallel simulations of sys-3. Related to Figure 1.

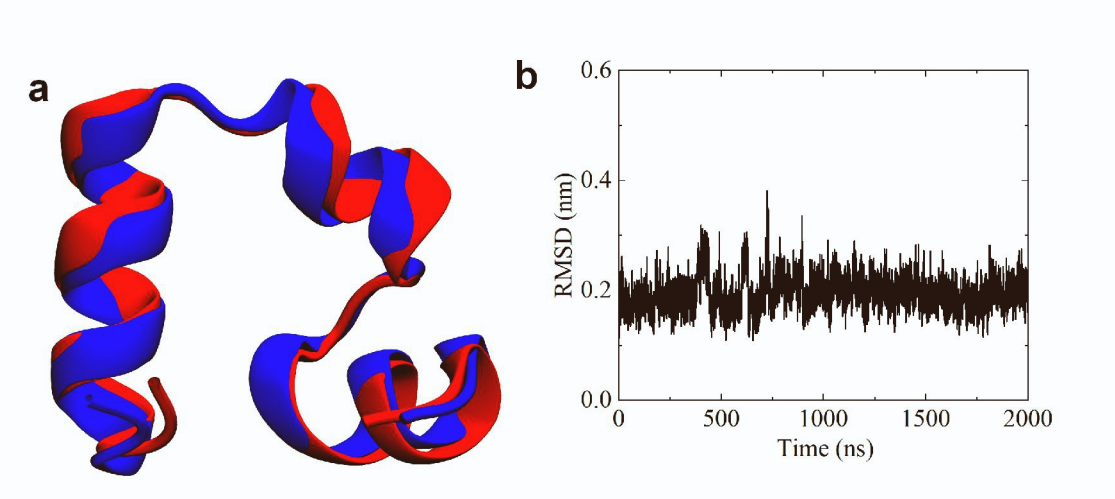

Figure S2. Simulation of an individual HP35 in absence of boridene. (a) Original (red) and final (blue) conformations of HP35 during a 2000-ns simulation. (b) RMSD of HP35 during the simulation. Related to Figure 1.

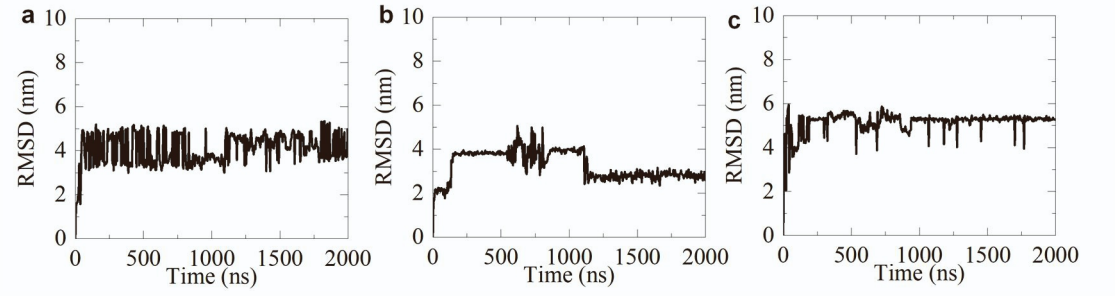

Figure S3. RMSD of HP35 versus boridene in three simulations of sys-1. Related to Figure 2.

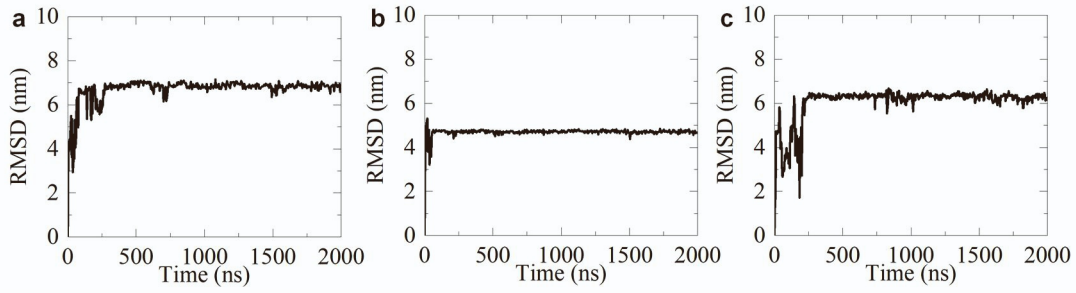

Figure S4. RMSD of HP35 versus boridene in three simulations of sys-2. Related to Figure 2.

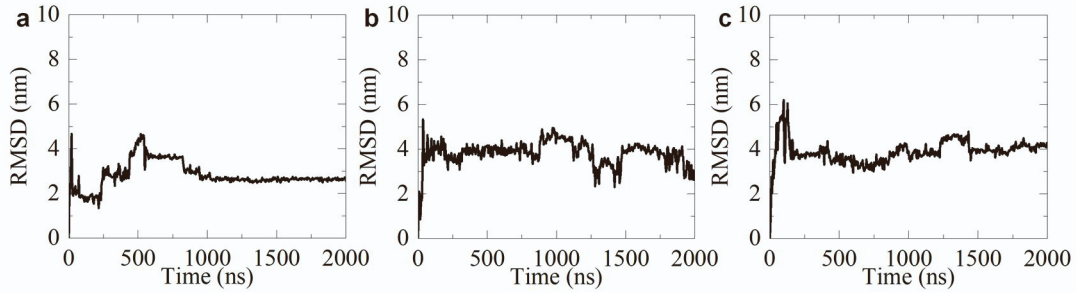

Figure S5. RMSD of HP35 versus boridene in three simulations of sys-3. Related to Figure 2.

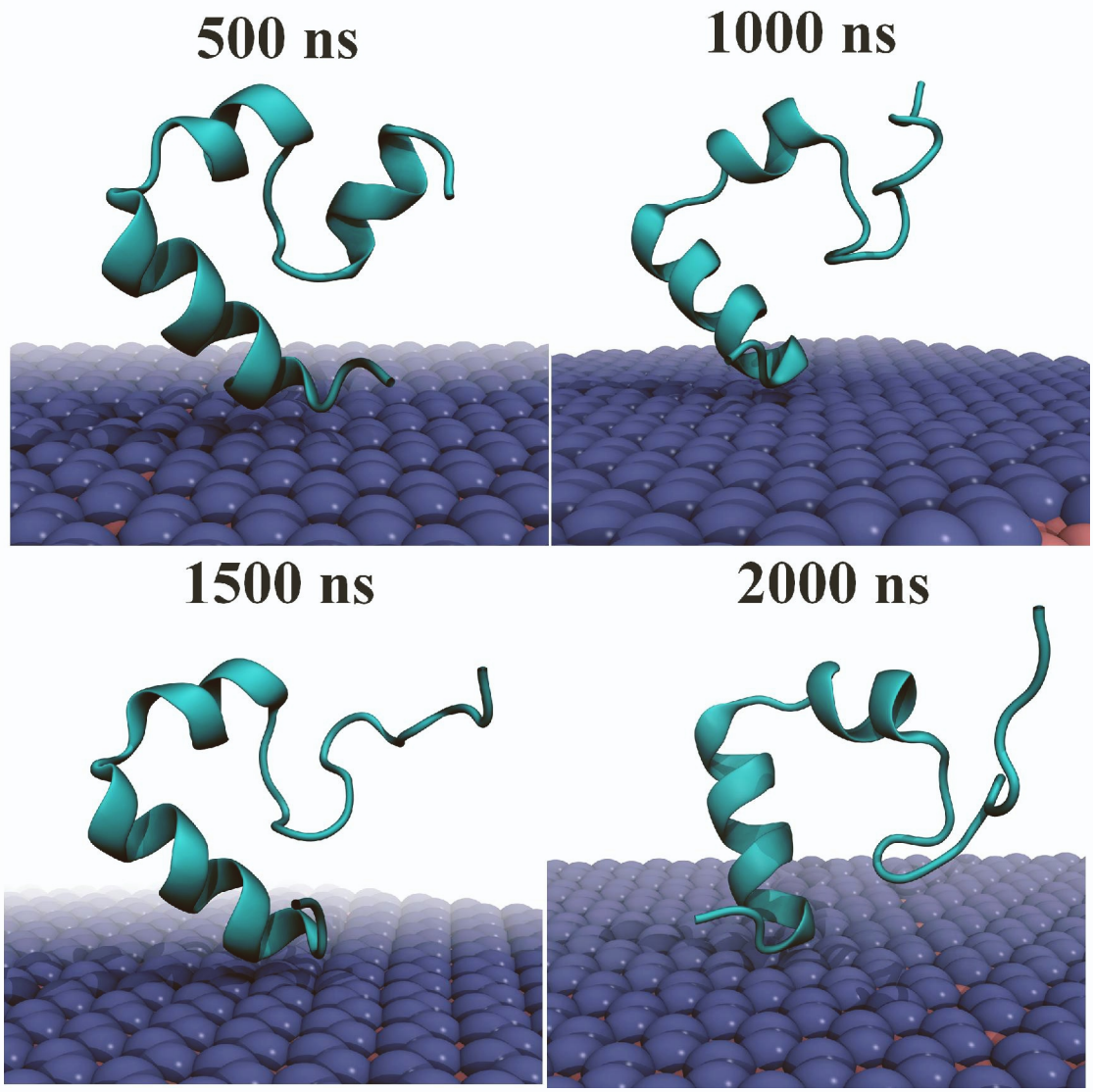

Figure S6. Snapshots of HP35 on boridene at four time points in the first simulation of sys-1. Related to Figure 2.

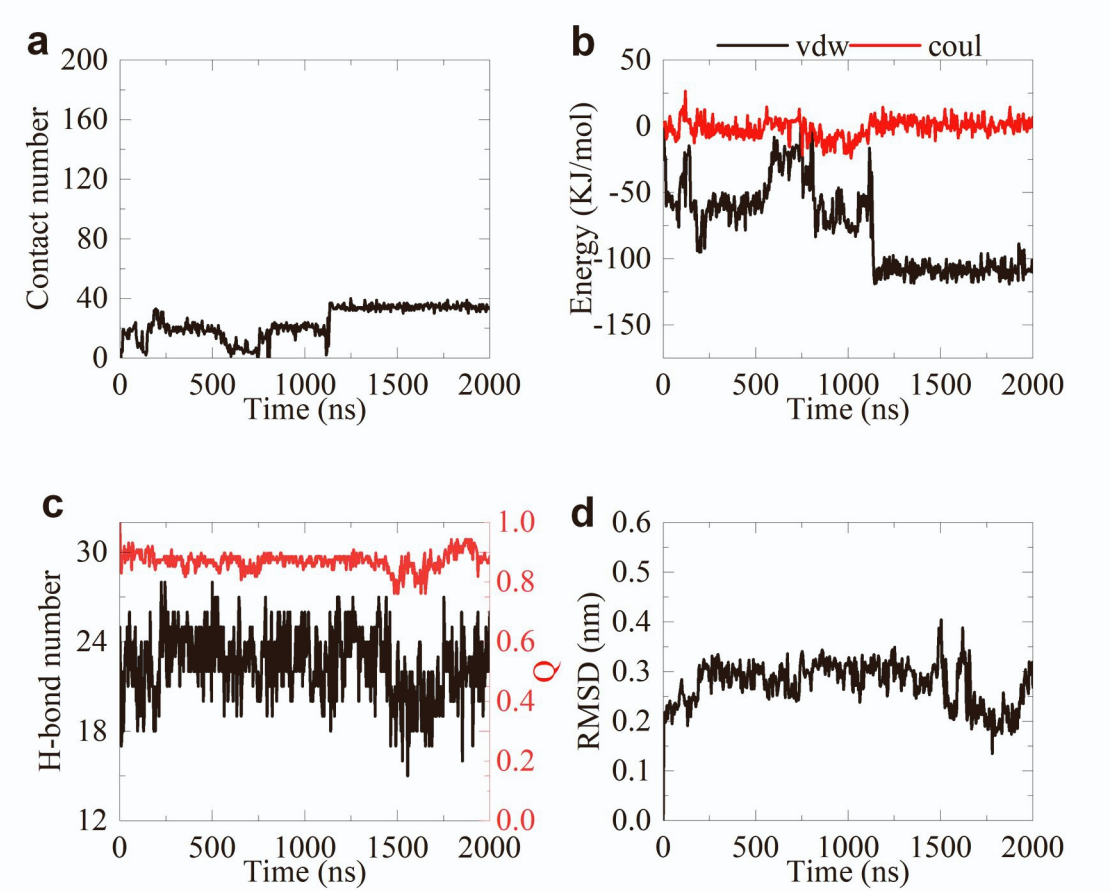

Figure S7. Binding kinetics of HP35 to boridene nanosheet in the second trajectory of sys-1 simulations. (a) Atom contact number of HP35 to boridene. (b) Interaction energies, including van der Waals (vdW) and Coulomb (Coul) energies, between HP35 and boridene. (c) Hydrogen bond (H-bond) number and Q value evolutions of HP35. (d) Root-mean-square displacement (RMSD) of HP35. Related to Figure 2.

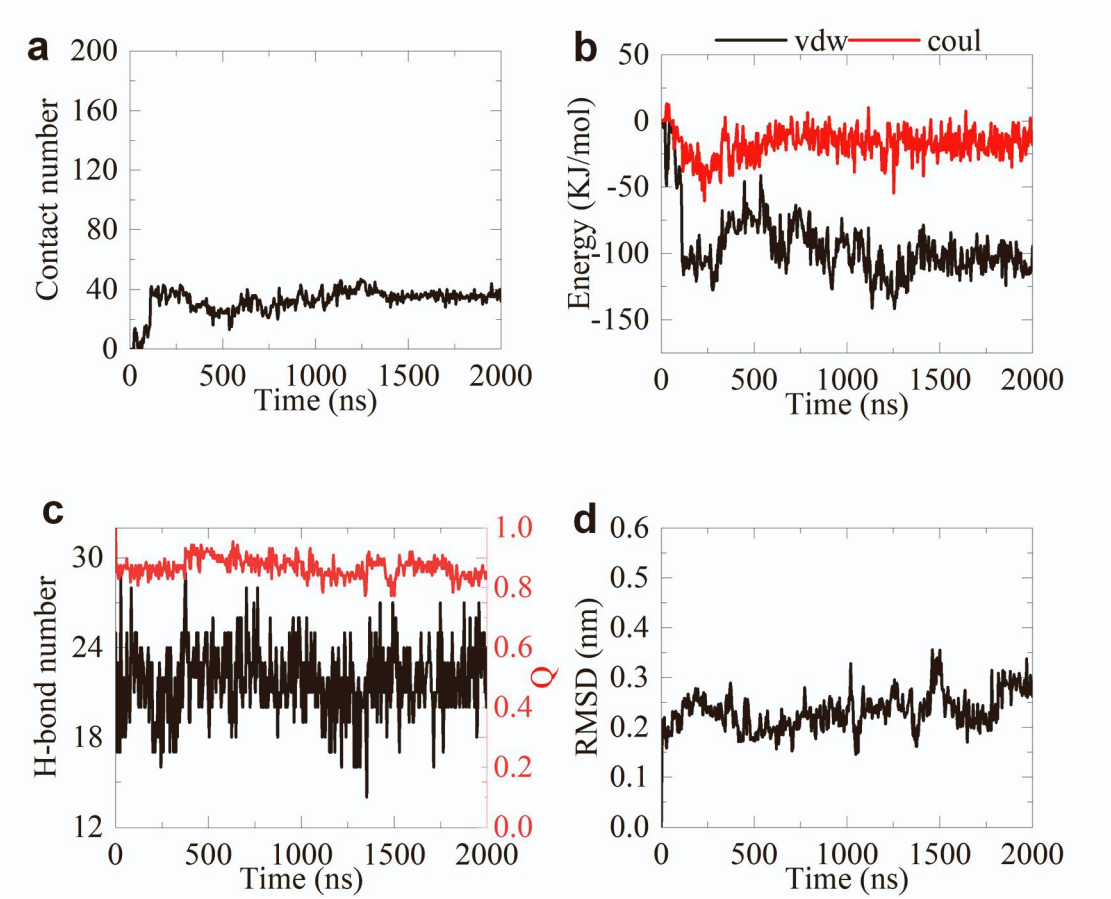

Figure S8. Binding kinetics of HP35 to boridene nanosheet in the third trajectory of sys-1 simulations. (a) Atom contact number of HP35 to boridene. (b) Interaction energies, including van der Waals (vdW) and Coulomb (Coul) energies, between HP35 and boridene. (c) Hydrogen bond (H-bond) number and Q value evolutions of HP35. (d) Root-mean-square displacement (RMSD) of HP35. Related to Figure 2.

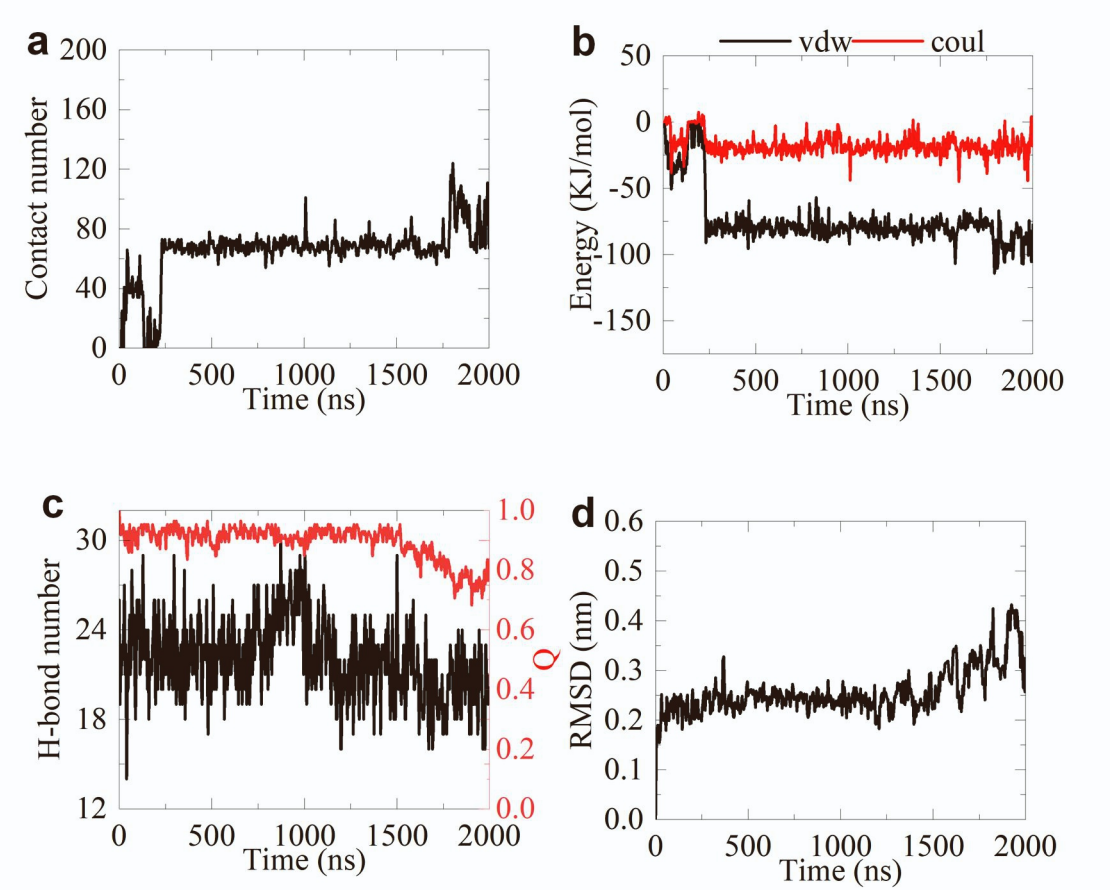

Figure S9. Binding kinetics of HP35 to boridene nanosheet in the first trajectory of sys-2 simulations. (a) Atom contact number of HP35 to boridene. (b) Interaction energies, including van der Waals (vdW) and Coulomb (Coul) energies, between HP35 and boridene. (c) Hydrogen bond (H-bond) number and Q value evolutions of HP35. (d) Root-mean-square displacement (RMSD) of HP35. Related to Figure 2.

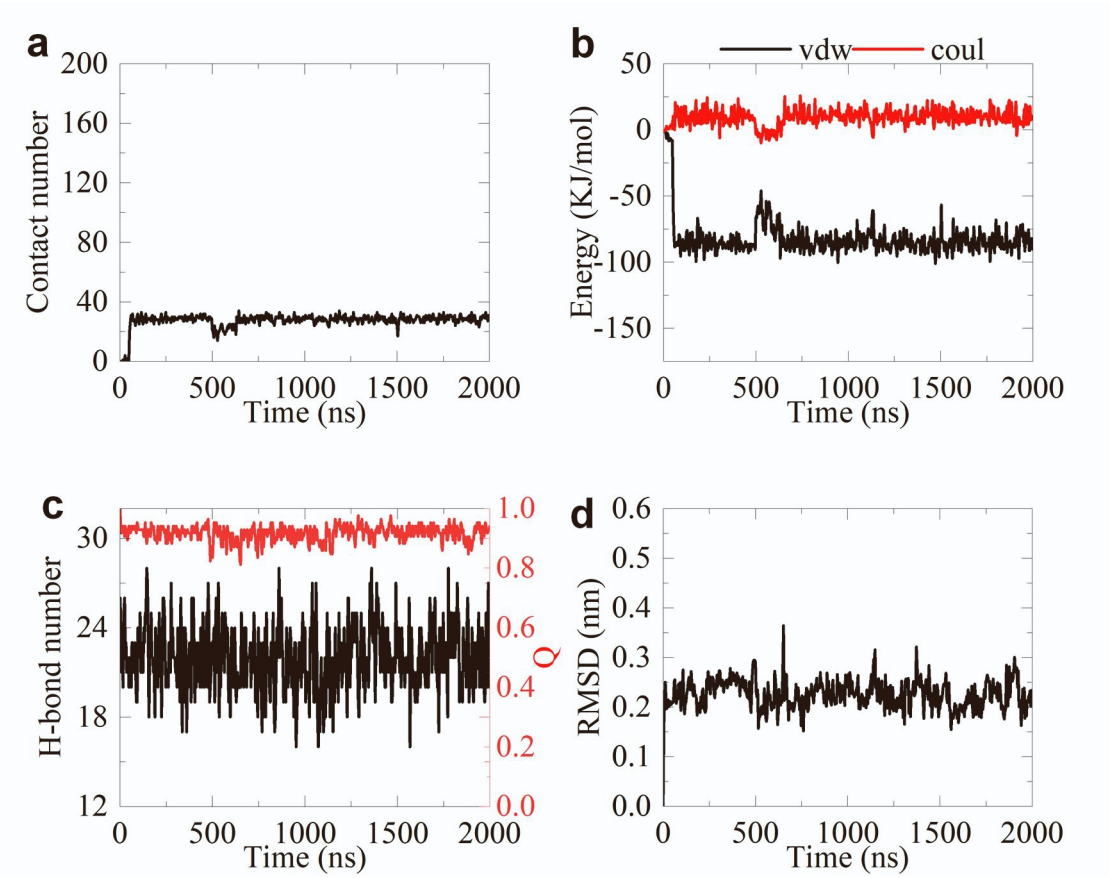

Figure S10. Binding kinetics of HP35 to boridene nanosheet in the second trajectory of sys-2 simulations. (a) Atom contact number of HP35 to boridene. (b) Interaction energies, including van der Waals (vdW) and Coulomb (Coul) energies, between HP35 and boridene. (c) Hydrogen bond (H-bond) number and Q value evolutions of HP35. (d) Root-mean-square displacement (RMSD) of HP35. Related to Figure 2.

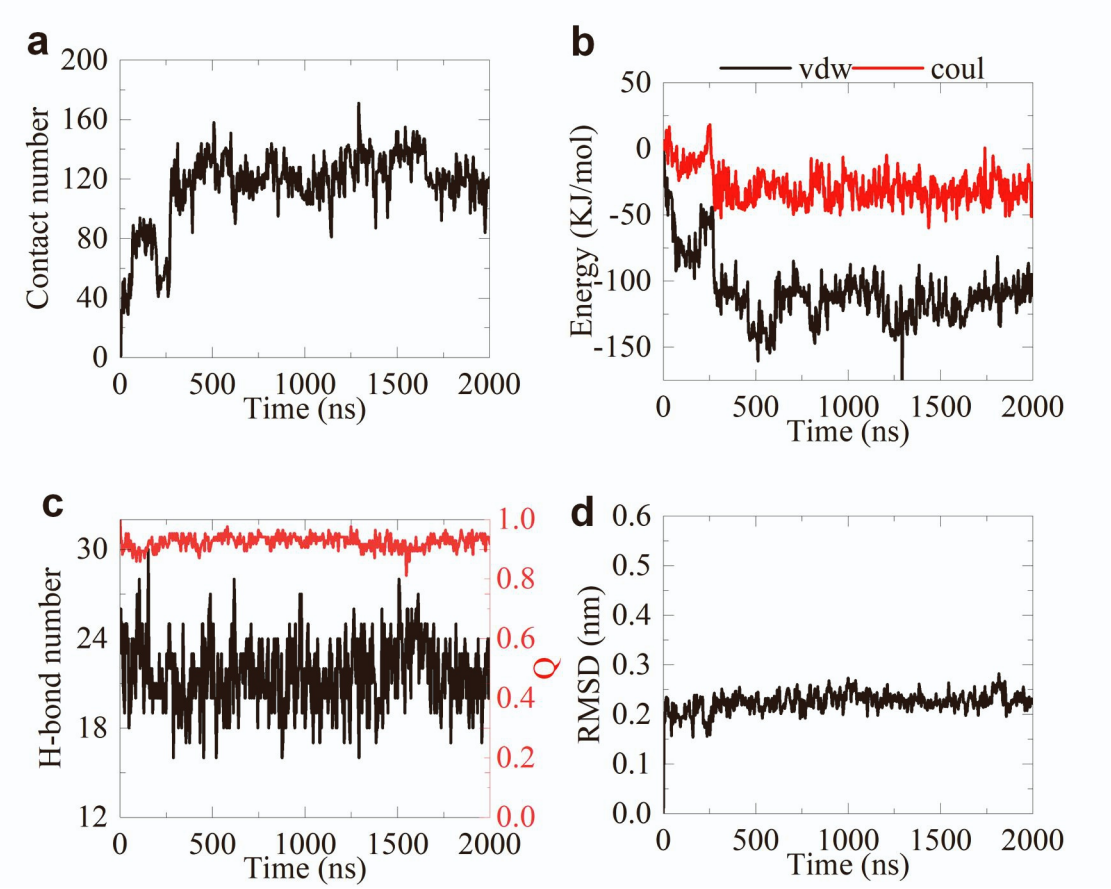

Figure S11. Binding kinetics of HP35 to boridene nanosheet in the third trajectory of sys-2 simulations. (a) Atom contact number of HP35 to boridene. (b) Interaction energies, including van der Waals (vdW) and Coulomb (Coul) energies, between HP35 and boridene. (c) Hydrogen bond (H-bond) number and Q value evolutions of HP35. (d) Root-mean-square displacement (RMSD) of HP35. Related to Figure 2.

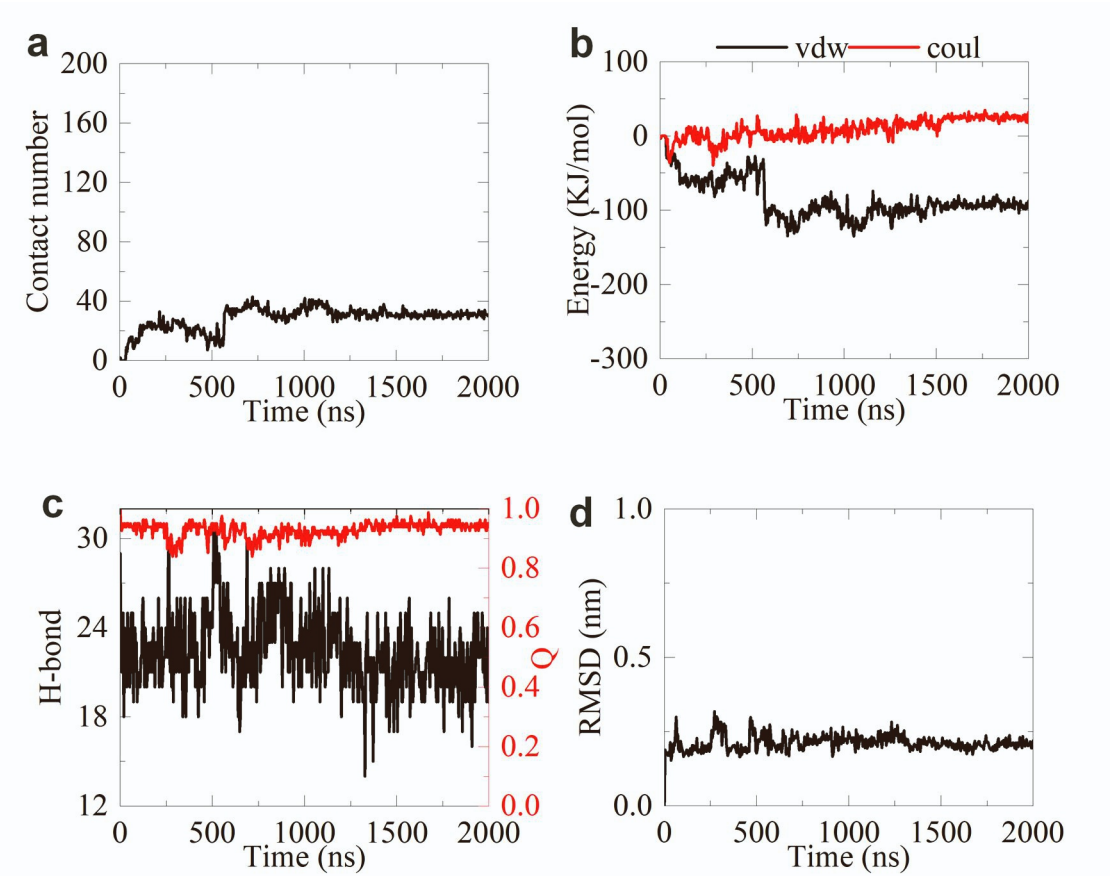

Figure S12. Binding kinetics of HP35 to boridene nanosheet in the first trajectory of sys-3 simulations. (a) Atom contact number of HP35 to boridene. (b) Interaction energies, including van der Waals (vdW) and Coulomb (Coul) energies, between HP35 and boridene. (c) Hydrogen bond (H-bond) number and Q value evolutions of HP35. (d) Root-mean-square displacement (RMSD) of HP35. Related to Figure 2.

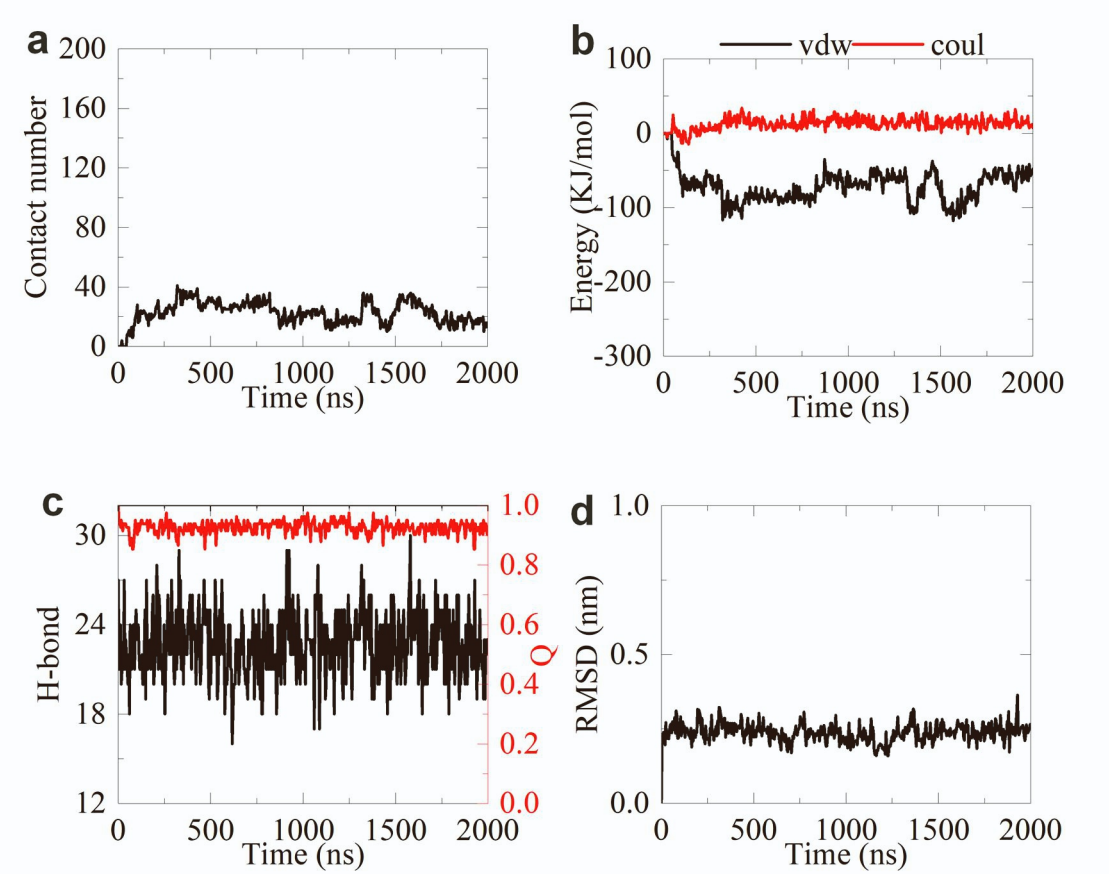

Figure S13. Binding kinetics of HP35 to boridene nanosheet in the second trajectory of sys-3 simulations. (a) Atom contact number of HP35 to boridene. (b) Interaction energies, including van der Waals (vdW) and Coulomb (Coul) energies, between HP35 and boridene. (c) Hydrogen bond (H-bond) number and Q value evolutions of HP35. (d) Root-mean-square displacement (RMSD) of HP35. Related to Figure 2.

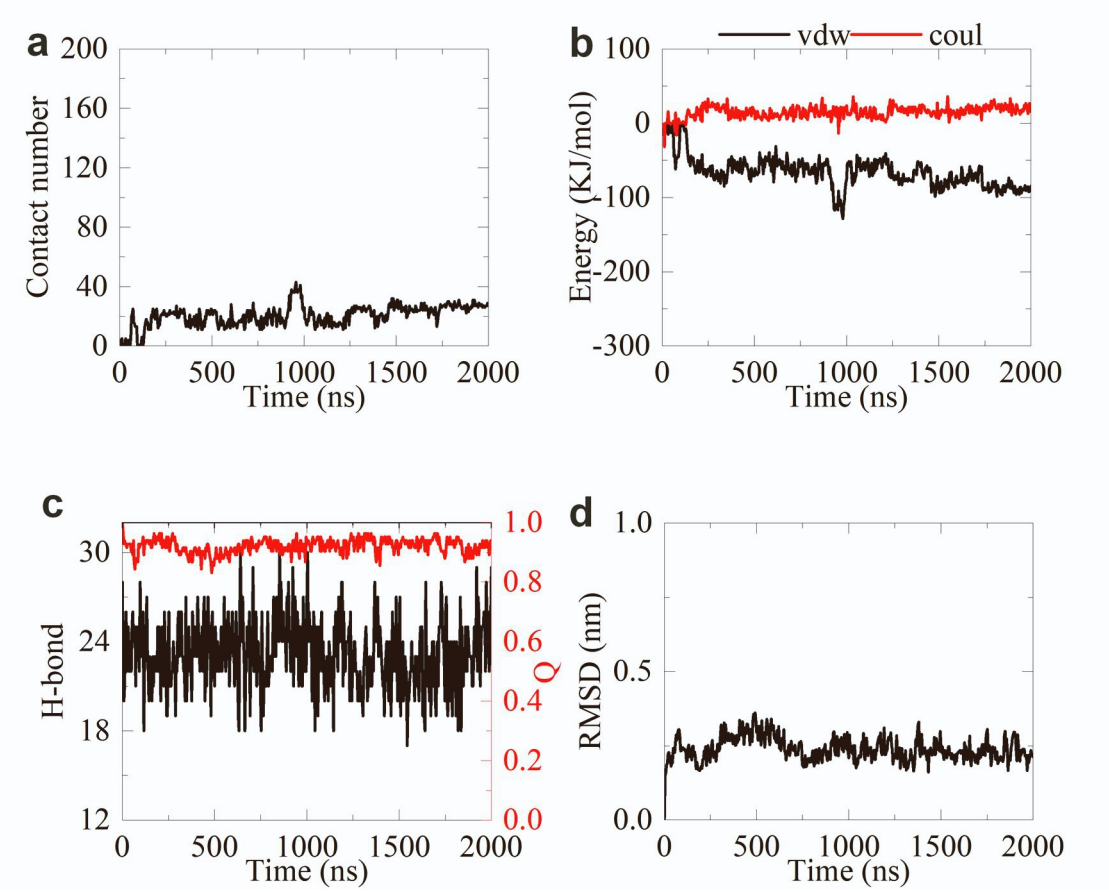

Figure S14. Binding kinetics of HP35 to boridene nanosheet in the third trajectory of sys-3 simulations. (a) Atom contact number of HP35 to boridene. (b) Interaction energies, including van der Waals (vdW) and Coulomb (Coul) energies, between HP35 and boridene. (c) Hydrogen bond (H-bond) number and Q value evolutions of HP35. (d) Root-mean-square displacement (RMSD) of HP35. Related to Figure 2.

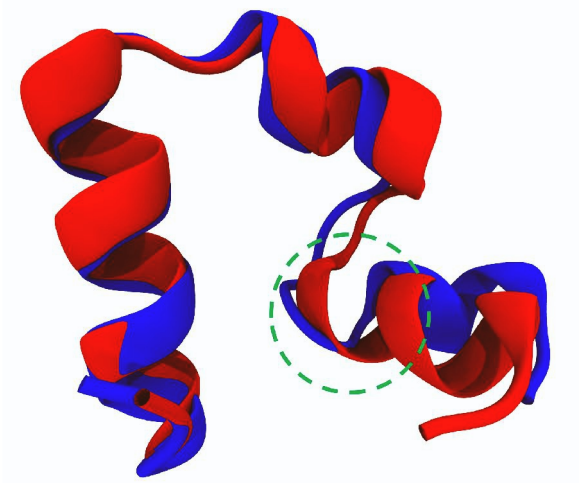

Figure S15. Unwinding region of HP35 in the first trajectory of sys-2 simulation. Red: Initial

HP35 structure; Blue: final HP35 structure. Green dashed circle indicates the local unwinding region.

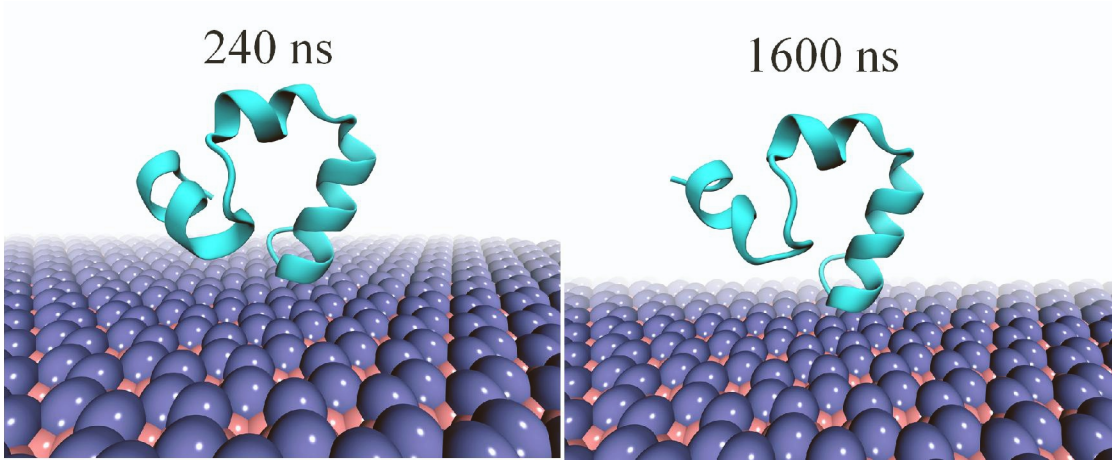

Figure S16. Snapshots showing the unfolding of HP35 on boridene in the first trajectory of sys-2 simulations. Related to Figure 2.

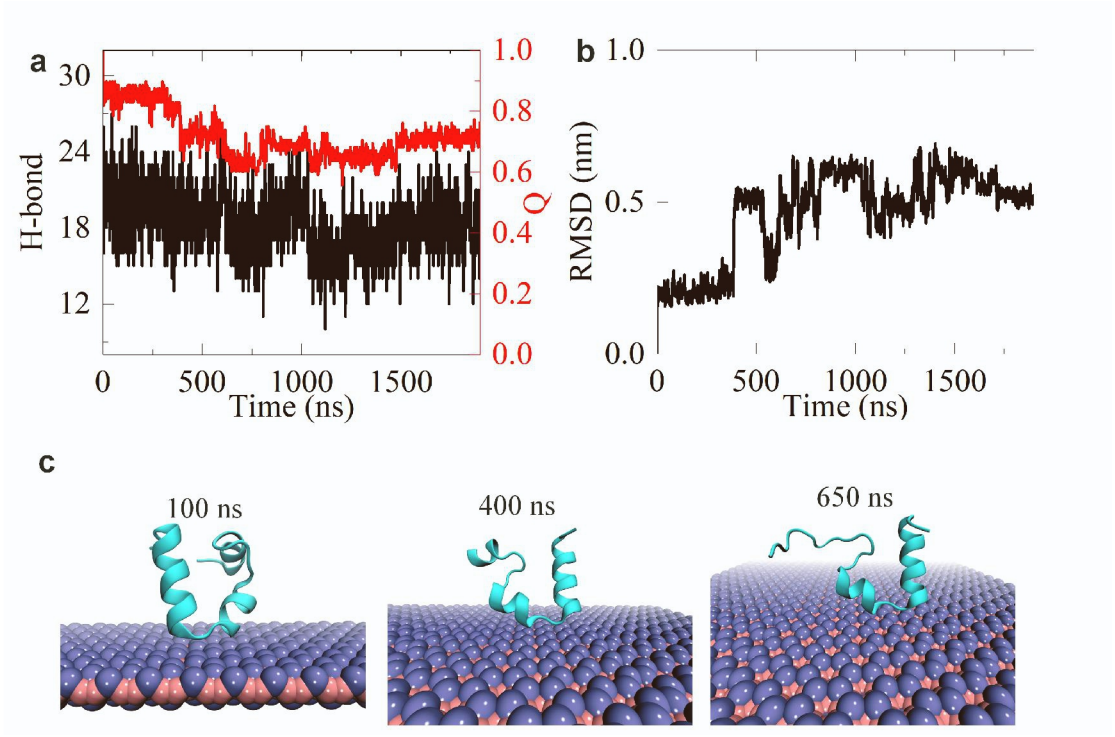

Figure S17. Unfolding of HP35 in an additional simulation of sys-1. (a) Hydrogen bond (H-bond) number and Q value evolutions of HP35. (b) Root-mean-square displacement (RMSD) of HP35.

(c) Three typical snapshots showing the unfolding process. Related to Figure 2.

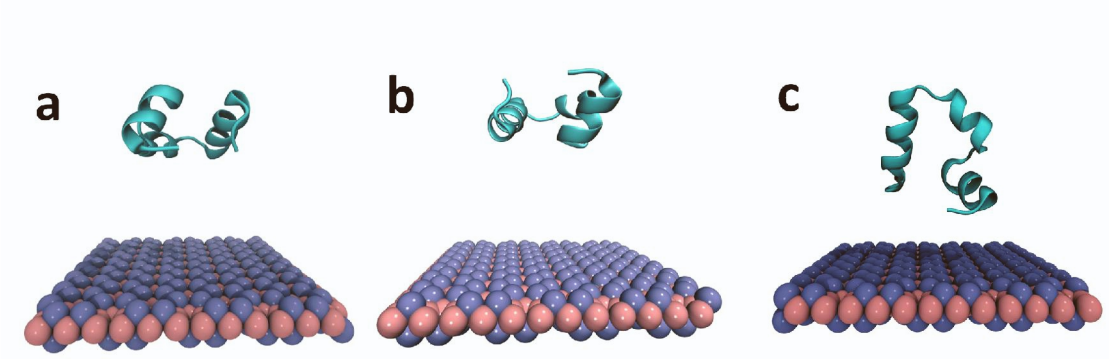

Figure S18. Initial conformations. In these three conformations, the HP35 rotates for 0° (a), 180° (b) and 270° (c) aiming at achieving the different initial structure, wherein HP35 faces to boridene with different surfaces. Related to STAR Methods.

Table S1. Simulation details of each system. Related to STAR Methods.

	box size (nm^3)	water number	Na^+ number	Cl^- number
sys-1	3.5×4.2×6	2372	8	10
sys-2	3.5×4.2×6	2377	8	10
sys-3	3.5×4.2×6	2465	8	10

Table S2. Force field parameters of boridene. Related to STAR Methods.

	σ (nm)	ε (kJ/mol)	charge (e)
molybdenum	0.415	0.7	0.405
boron	0.24	0.5	-0.27

Table S3. Optimized coordinates of boridene segment. Related to STAR Methods.

CRYST1	5.176	8.964	17.697	89.39	90.31	90.00 P 1			1		
ATOM	1	B1	MOL X	2	2.839	1.995	8.210	1.00	0.01		B
ATOM	2	B2	MOL X	2	1.972	0.494	8.206	1.00	0.01		B
ATOM	3	B3	MOL X	2	2.824	7.978	8.214	1.00	0.01		B

```
ATOM      4  B4   MOL X   2       1.958   6.477   8.210  1.00  0.01           B
ATOM      5  B5   MOL X   2       0.251   6.477   8.210  1.00  0.01           B
ATOM      6  B6   MOL X   2       4.560   4.976   8.207  1.00  0.01           B
ATOM      7  B7   MOL X   2       0.236   3.496   8.214  1.00  0.01           B
ATOM      8  B8   MOL X   2       2.824   4.976   8.206  1.00  0.01           B
ATOM      9  B9   MOL X   2       1.973   3.496   8.212  1.00  0.01           B
ATOM     10  B10  MOL X   2       0.237   0.494   8.205  1.00  0.01           B
ATOM     11  B11  MOL X   2       4.560   7.978   8.212  1.00  0.01           B
ATOM     12  B12  MOL X   2       4.546   1.994   8.210  1.00  0.01           B
ATOM     13  Mo1  MOL X   2       3.692   6.466   9.653  1.00  0.01          MO
ATOM     14  Mo2  MOL X   2       1.104   2.007   6.766  1.00  0.01          MO
ATOM     15  Mo3  MOL X   2       3.692   3.494   9.616  1.00  0.01          MO
ATOM     16  Mo4  MOL X   2       1.104   4.978   6.804  1.00  0.01          MO
ATOM     17  Mo5  MOL X   2       1.104   1.984   9.653  1.00  0.01          MO
ATOM     18  Mo6  MOL X   2       3.692   6.488   6.766  1.00  0.01          MO
ATOM     19  Mo7  MOL X   2       1.104   7.976   9.615  1.00  0.01          MO
ATOM     20  Mo8  MOL X   2       3.692   0.495   6.803  1.00  0.01          MO
END
```