

## Supporting Information

# Molecular-level understanding of the adsorption mechanism of a graphite-binding peptide at the water/graphite interface

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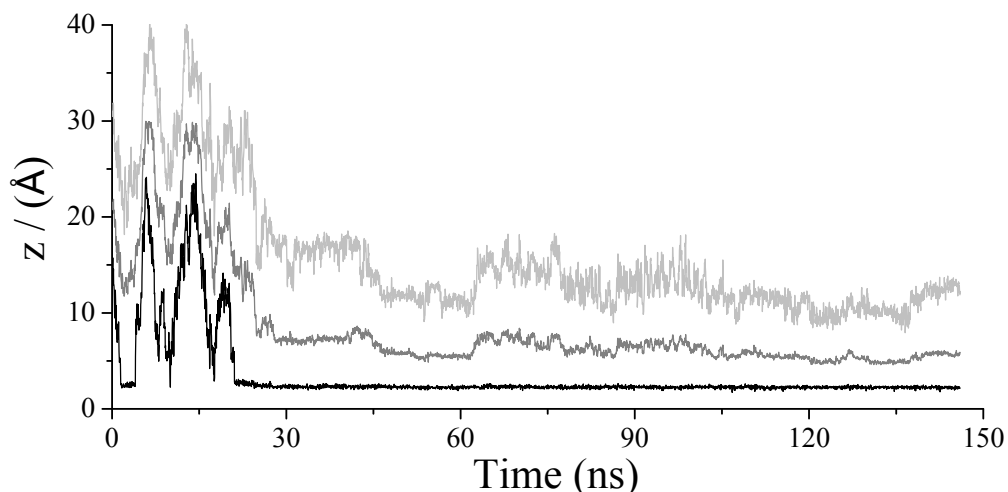
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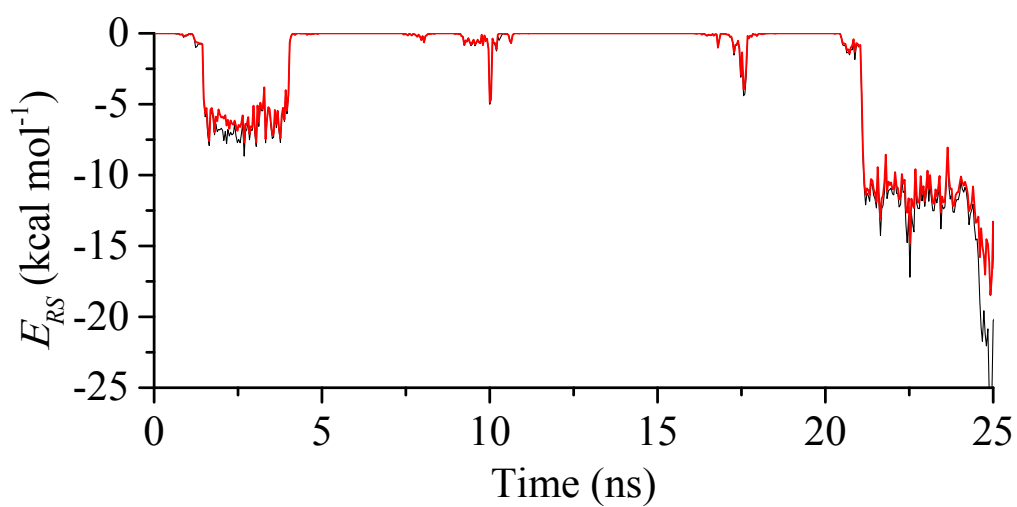
## 1. Additional relevant results and analysis.

### 1.1 Full trajectory for exemplar run.



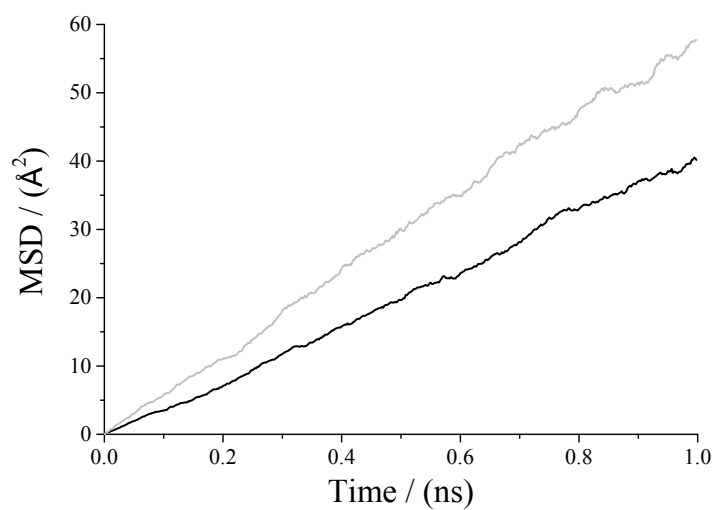
**Figure S1.** Full trajectory for the exemplar run subdivided into Figure 3, Figure 4 and Figure 5. SSD<sub>MIN</sub> (black), SSD<sub>COM</sub> (dark grey), SSD<sub>MAX</sub> (light gray).

## 1.2 Peptide-surface interaction energy for exemplar run.



**Figure S2.** Total interaction energy between peptide and surface,  $E_{PS}$ , (black) and the interaction energy between residues Ile<sub>1</sub>, Tyr<sub>9</sub> and Tyr<sub>12</sub> and the surface (red).

## 1.3 MSD data.



**Figure S3.** MSD for GrBP5 in the adsorbed (black) and bulk (light gray) states.