

# Supporting Information for Detection and Mapping of DNA Methylation with 2D Material Nanopores

Hu Qiu,<sup>†,||</sup> Aditya Sarathy,<sup>†,‡,||</sup> Klaus Schulten,<sup>\*,†,¶</sup> and Jean-Pierre Leburton<sup>\*,†,¶,§</sup>

<sup>†</sup>*Beckman Institute for Advanced Science and Technology*

<sup>‡</sup>*Department of Electrical and Computer Engineering*

<sup>¶</sup>*Department of Physics*

<sup>§</sup>*Department of Electrical and Computer Engineering, University of Illinois, Urbana, Illinois 61801, United States*

<sup>||</sup>*Contributed equally to this work*

E-mail: [kschulte@ks.uiuc.edu](mailto:kschulte@ks.uiuc.edu); [jleburto@illinois.edu](mailto:jleburto@illinois.edu)

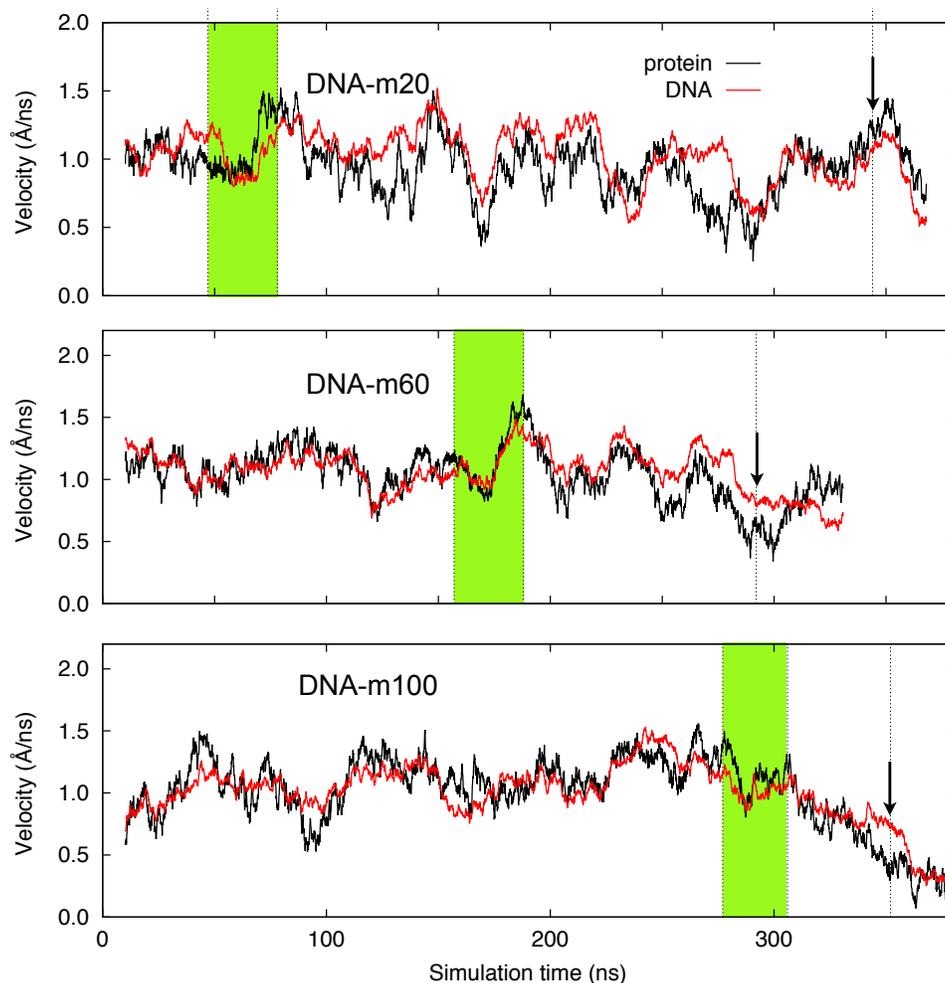


Figure S1: Velocity of the center of mass of DNA (red) and protein (black) when three mDNA-MBD1 complexes, formed based on mDNA with a single methylation site present in three different positions: 20th (top), 60th (middle), and 100th (bottom) bp, are translocated through a 5 nm graphene nanopore. The green rectangles highlight the time duration when the MBD1 protein resides in the pore and the arrows denote the time instant when the complex leaves the pore.

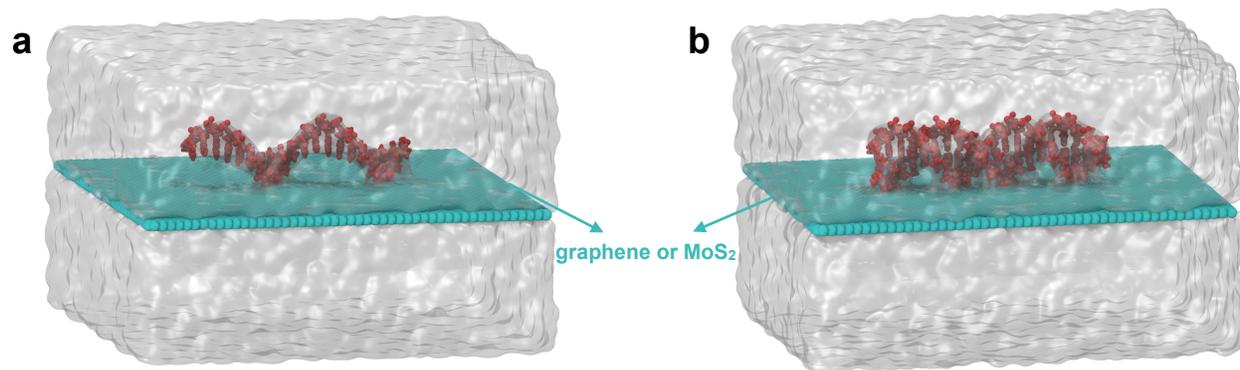


Figure S2: Simulation system of a ssDNA A20 (a) and a dsDNA AT20 (b) adsorbed onto a graphene or MoS<sub>2</sub> surface. Initially, the axis of DNA was aligned parallel to the surface, with a DNA-surface separation of 0.1 nm.

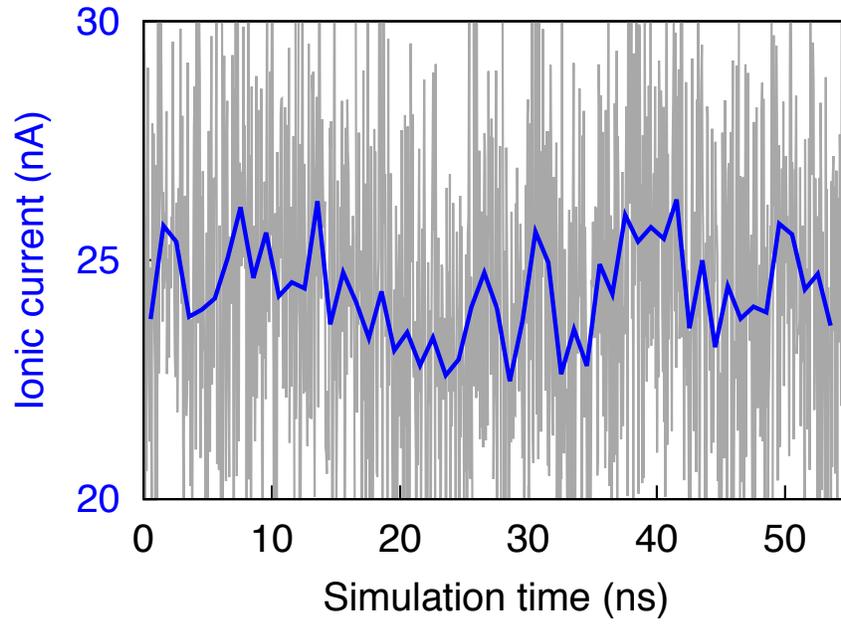


Figure S3: Ionic current trace as a mDNA-MBD1 complex is translocated through a 8 nm diameter MoS<sub>2</sub> nanopore under a voltage of 0.5 V. No significant dip for the MBD1 is observed.