Supporting information for:

Molecular Dynamics Simulation of Water Transport Mechanisms through Nanoporous Boron Nitride and Graphene Multilayers

Majid Shahbabaei, and Daejoong Kim*

Department of Mechanical Engineering, Sogang University, Seoul 121-742, Republic of Korea

daejoong@sogang.ac.kr

Postal address: 35 Baekbeom-ro, Mapo-gu, Seoul, Republic of Korea, 121-742

Phone number: (+82) 2-705-8644

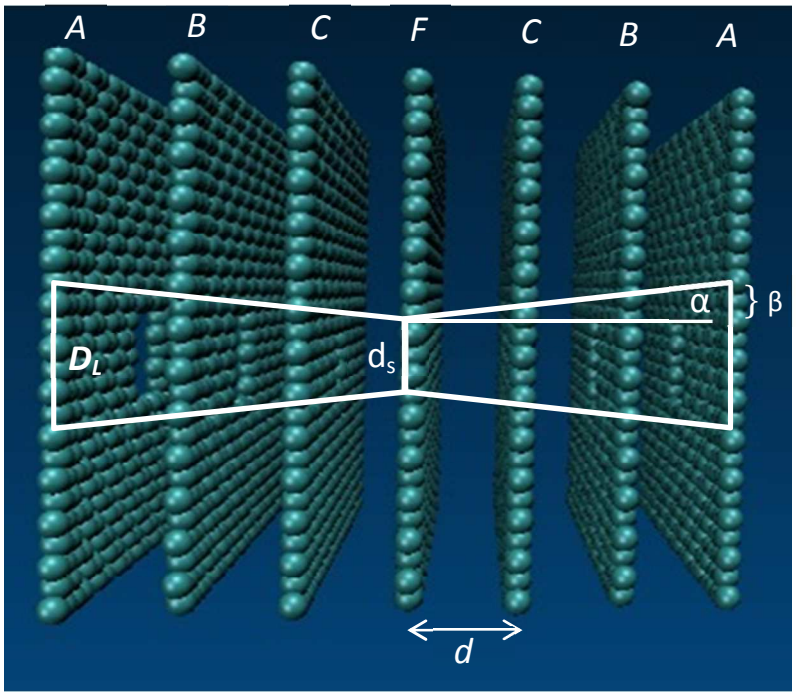

Figure S1. Schematic of an hourglass-shaped nanopore in multilayer structure. All the nanopore models are symmetrical with the same effective pore diameter in layers A, B, and C, respectively. D_L, d_S, d and α are the largest diameter (constant at 8 Å), narrowest diameter (constant at 5 Å), interlayer distance, and the cone angle of hourglass-shaped structure, respectively. Using the relation $tan\alpha=\beta/d$, the cone angle α can be determined. Next, using the cone angle and changing the interlayer distance, the diameter of the pores located in layers B and C can be estimated.

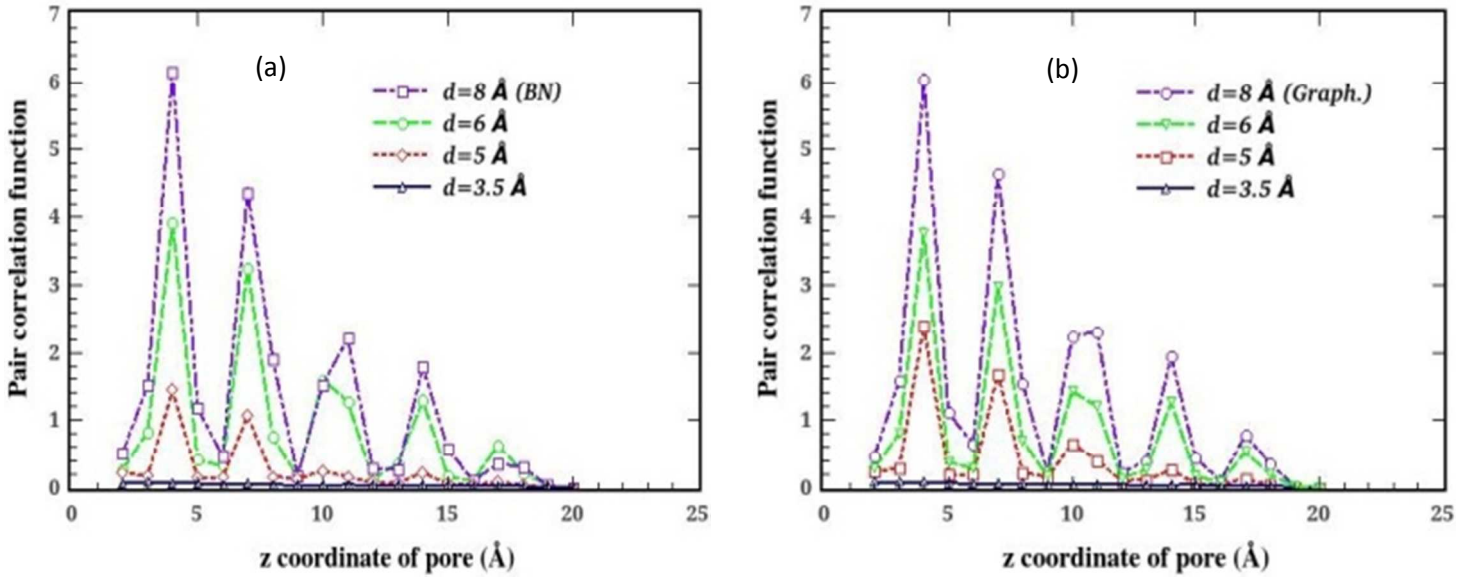

Figure S2. Pair correlation function of water molecules inside (a) boron nitride (BN) and (b) graphene with variation of layer separation.

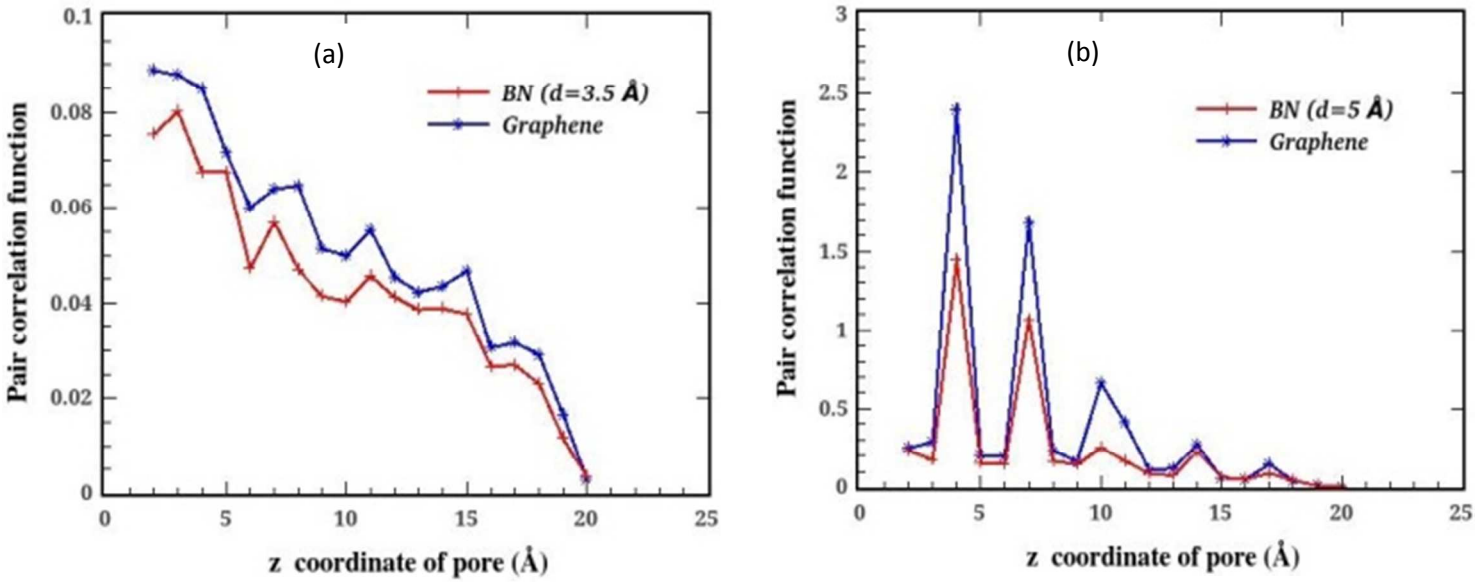

Figure S3. Pair correlation function of water molecules inside boron nitride (BN) and graphene with layer separation of (a) 3.5 Å and (b) 5 Å.

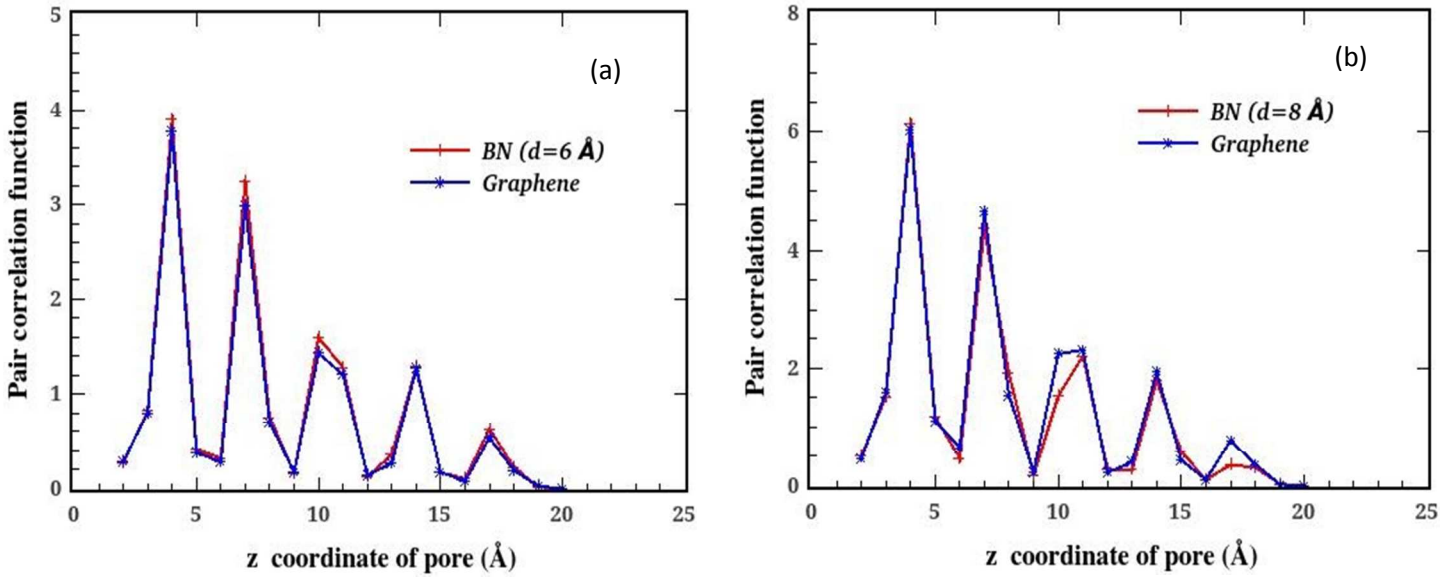

Figure S4. Pair correlation function of water molecules inside boron nitride (BN) and graphene with layer separation of (a) 6 Å and (b) 8 Å.