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Structure and Dynamic Properties of Stretched Water in Graphene Nanochannels by Molecular Dynamics simulation: Effects of Stretching Extent

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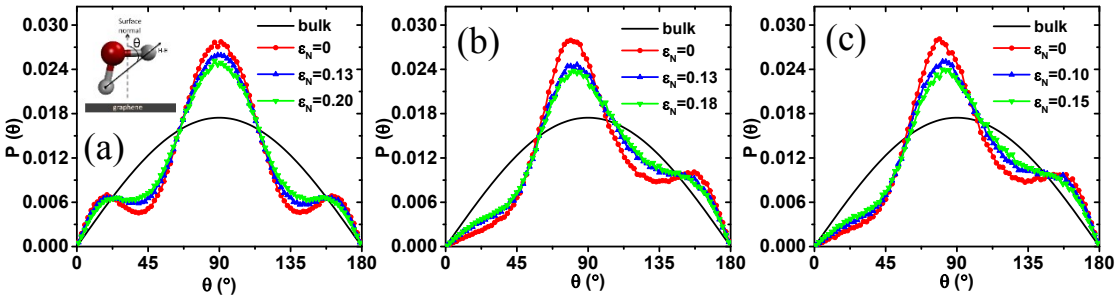

Fig. S1 The orientation distribution probability profiles of stretched water confined within various graphene channels at 300 K, respectively. The left, middle and right panels represent cases of L =1 nm (a), L = 2 nm (b) and L = 3 nm (c), respectively. Black solid lines represent the results of bulk water.

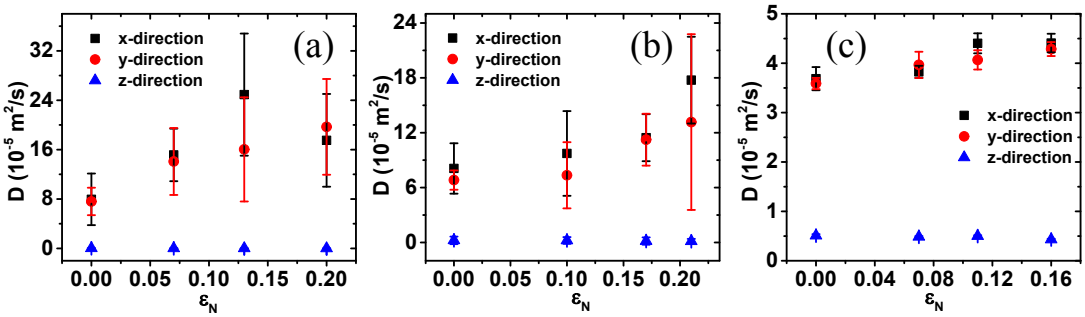

Fig. S2 The self-diffusion coefficient in x, y and z directions of confined water under stretching within L =1 nm (a), L = 2 nm (b) and L = 3 nm (c), respectively.

Table S1 The tangential and normal pressure tensor of water confined in graphene channels of different width at 300 K

L (nm)	Stretching coefficient(ε_N)	Number of water molecules(N)	P_T (10^3 bar)	P_N (10^3 bar)
1	0	224	−0.01931	0.338797
	0.07	209	−1.38103	−0.70625
	0.13	194	−2.0441	−1.19022
	0.20	179	−2.22324	−1.35588
2	0	576	−0.23104	0.643891
	0.06	515	−1.26623	−0.78248
	0.13	478	−1.52363	−1.14071
	0.18	452	−1.59709	−1.33046
3	0	885	−0.0412	0.532845
	0.05	838	−0.82055	−0.42521
	0.10	798	−1.29241	−1.00215
	0.15	753	−1.53774	−1.37229