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Breakdown of Continuum Model for Water Transport and Desalination through
Ultrathin Graphene Nanopores: Insights from Molecular Dynamics Simulations

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Table.S1. Forcefield for non-bonded interaction parameters of atoms in the system.

$$U_{LJ} = 4\varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right]$$

Molecule	Atom symbol	ε [kJ/mol]	σ [Å]
Membrane	C	0.293	3.4
Water	Ow	0.774	3.15
	Hw	0.000	1.00
NaCl salt	Na	0.012	3.33
	Cl	0.492	4.42

Table.S2. Forcefield parameters for bonded interaction of atoms in the system

$$U_{Bond} = K_b [b - b_o]^2$$
$$U_{Angle} = K_\theta [\theta - \theta_o]^2$$

Bonds	K_b [kJ/mol-Å^2]	Equilibrium bond length b_o [Å]
C-C	1960.42	1.420
Ow-Hw	1881.00	0.957
Angles	K_θ [kJ/mol-rad^2]	Equilibrium angle θ_o [degree]
C-C-C	263.34	120
Hw-Ow-Hw	229.9	104.52

Fig.S1. Stress correlation function of water confined in graphene nanopores vs. (i) pore size [P=150MPa, C=0.2M], (ii) external pressure [h=7Å, C=0.2M], and (iii) salt concentration [h=7Å, P=150MPa]

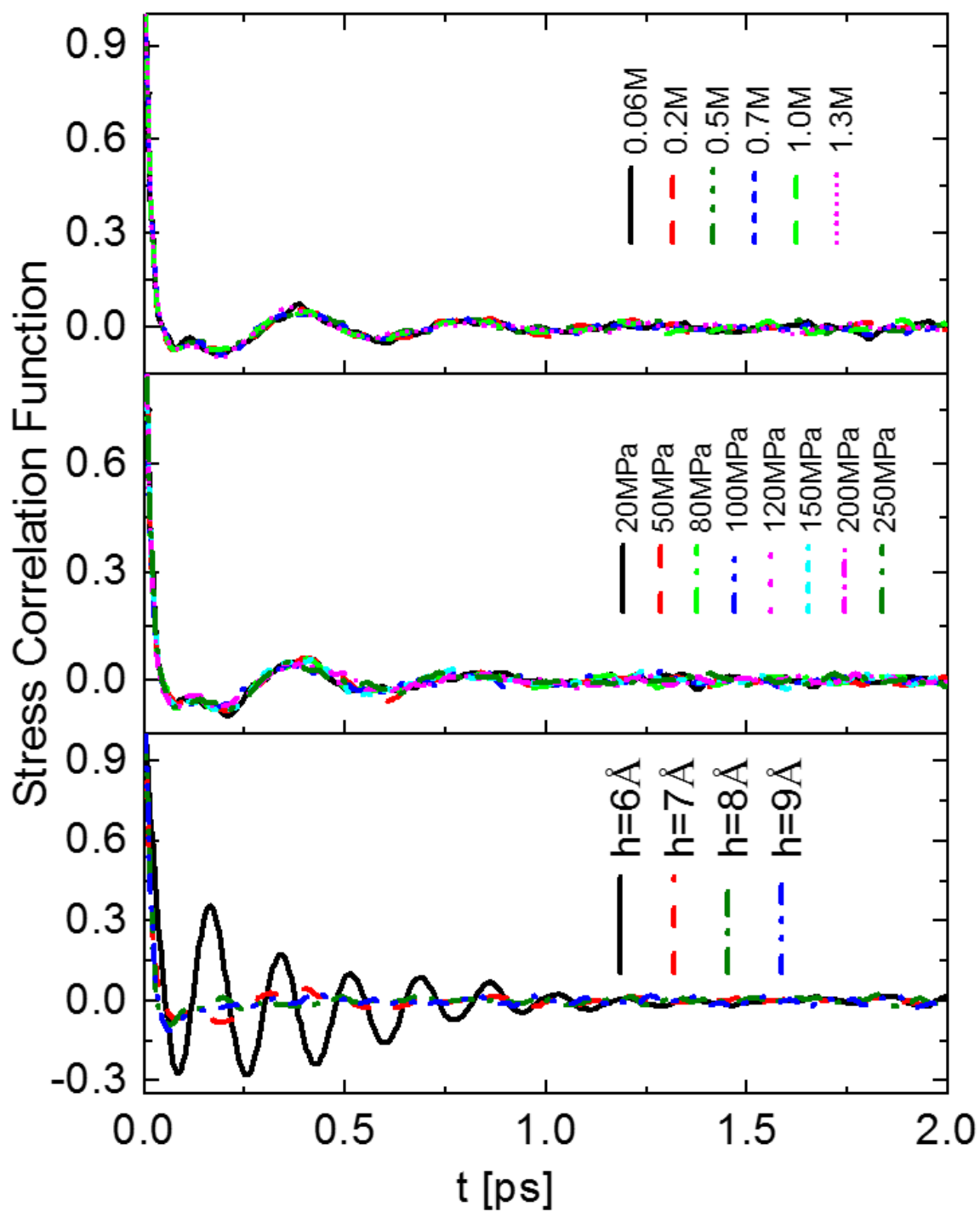**Fig.S2.** Force autocorrelation function of water confined in graphene nanopores vs. (i) pore size [P=150MPa, C=0.2M], (ii) external pressure [h=7Å, C=0.2M], and (iii) salt concentration [h=7Å, P=150MPa].

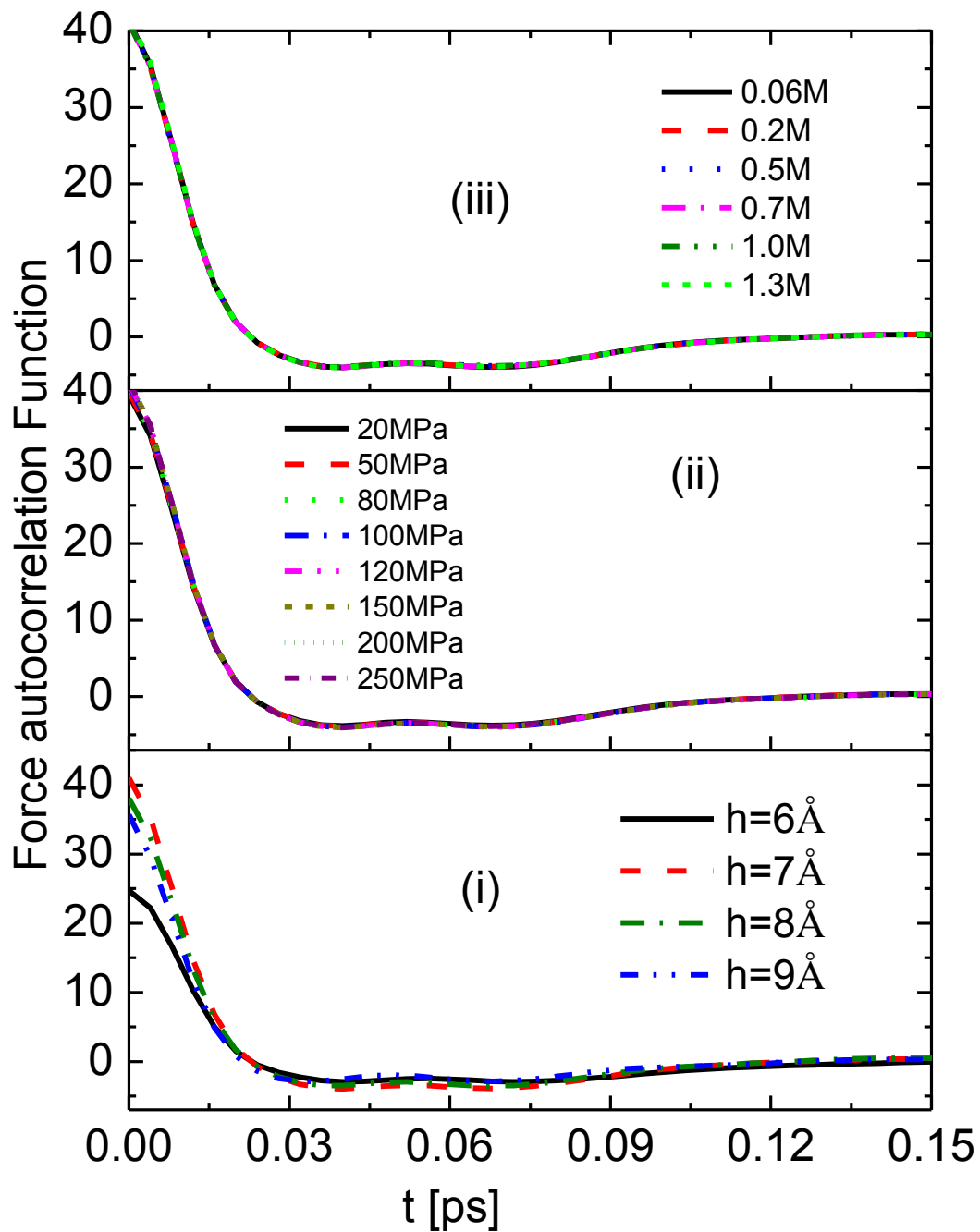**Fig.S3. Viscosity of water confined in graphene nanopores vs. (i) pore size [P=150MPa, C=0.2M], (ii) external pressure [h=7Å, C=0.2M], and (iii) salt concentration [h=7Å, P=150MPa]**
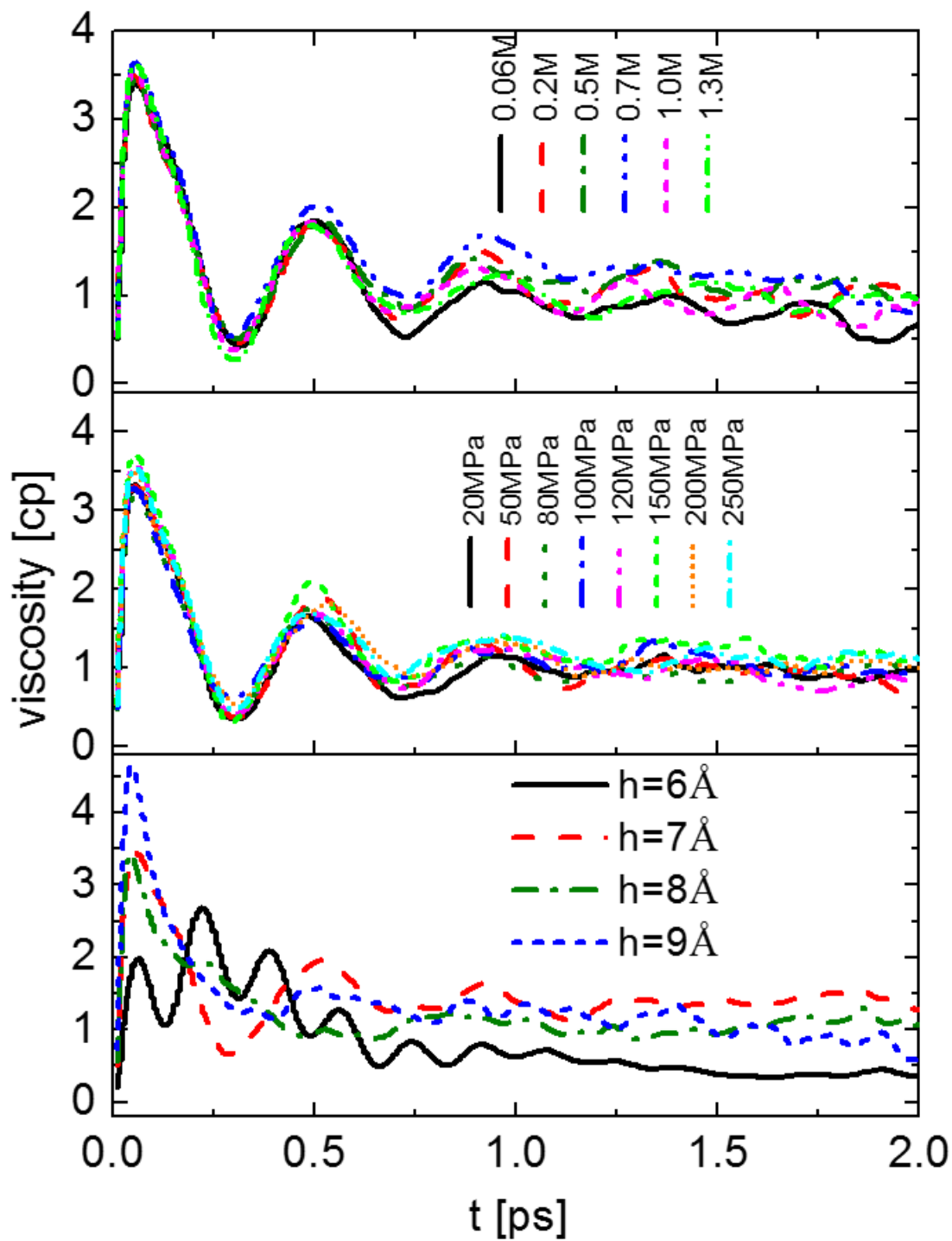
Fig.S4. Velocity autocorrelation function of water confined in graphene nanopores vs. (i) pore size [P=150MPa, C=0.2M], (ii) external pressure [h=7Å, C=0.2M], and (iii) salt concentration [h=7Å, P=150MPa].