

Supporting Information for

Exploring the contribution of charge species at outer surface to ion current signal of nanopores: a theoretical stud

Haowei Mao^a, Qun Ma^a, Hongquan Xu^a, Lei Xu^a, Qiujiào Du^b, Pengcheng Gao^{a, *}, Fan Xia^a

^aEngineering Research Center of Nano-Geomaterials of Ministry of Education, Faculty of Materials Science and Chemistry, China University of Geosciences, Wuhan 430074, P. R. China. ^bSchool of Mathematics and Physics, China University of Geosciences, Wuhan 430074, P. R. China.

* Correspondence to: pcgao@cug.edu.cn;

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1. Supplementary Figures

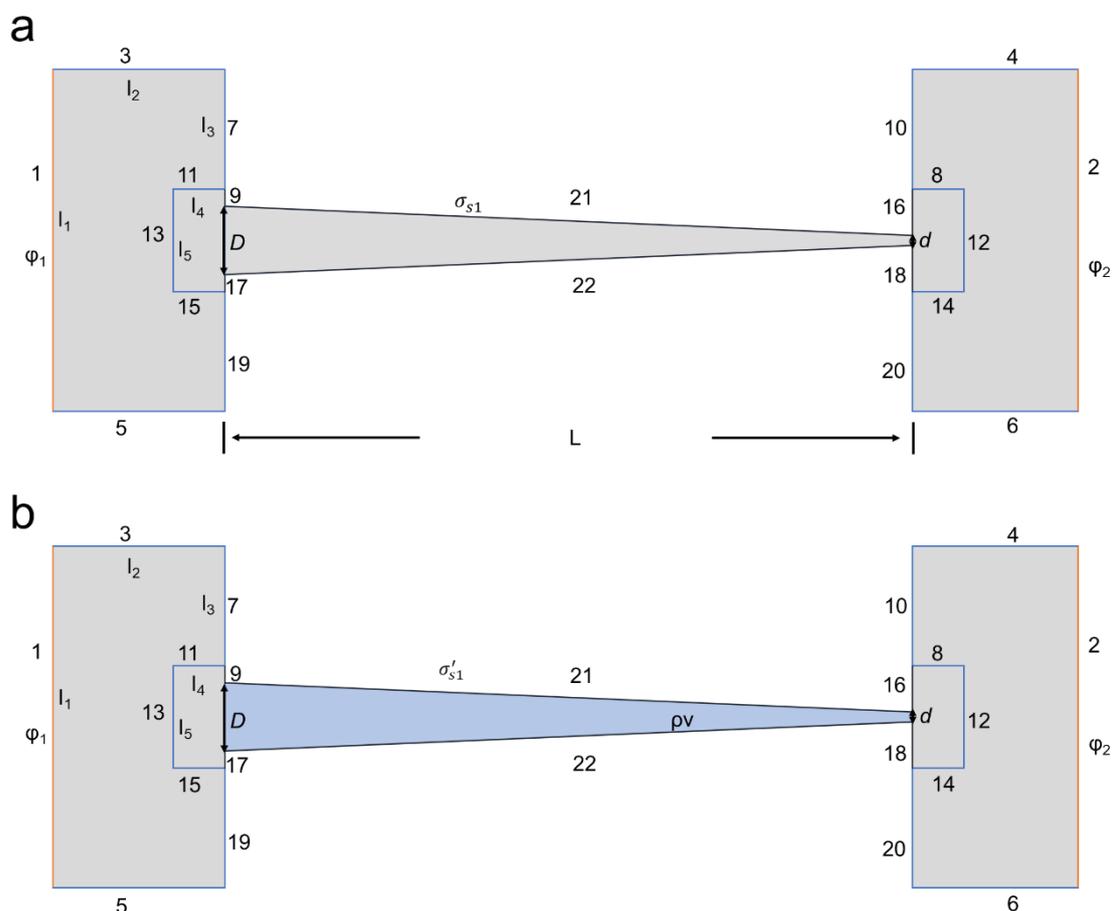


Figure S1. The models used in the numerical simulations.(a) Surface charge model and (b) space charge model. The ion transport model of Probe molecule modified nanopore controlled by surface charge and space charge is established by using multi physical field simulation software COMSOL. Both models contain a channel with length of 2000 nm, initial tip diameter of 25 nm and base diameter of 200nm. The system is filled with the electrolyte solution at the concentration. A voltage of -2 V is applied to both ends of the square area as the driving force for the ion transmission. The specific boundary conditions of the two models are shown in Table S1.

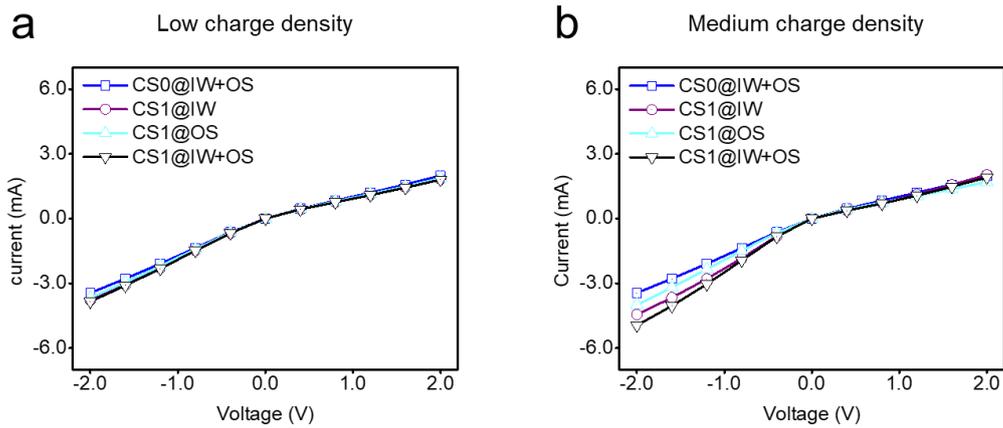


Figure S2. The I-V curves of different charge density.(a) I-V curves of low charge density. (b) I-V curves of medium charge density.

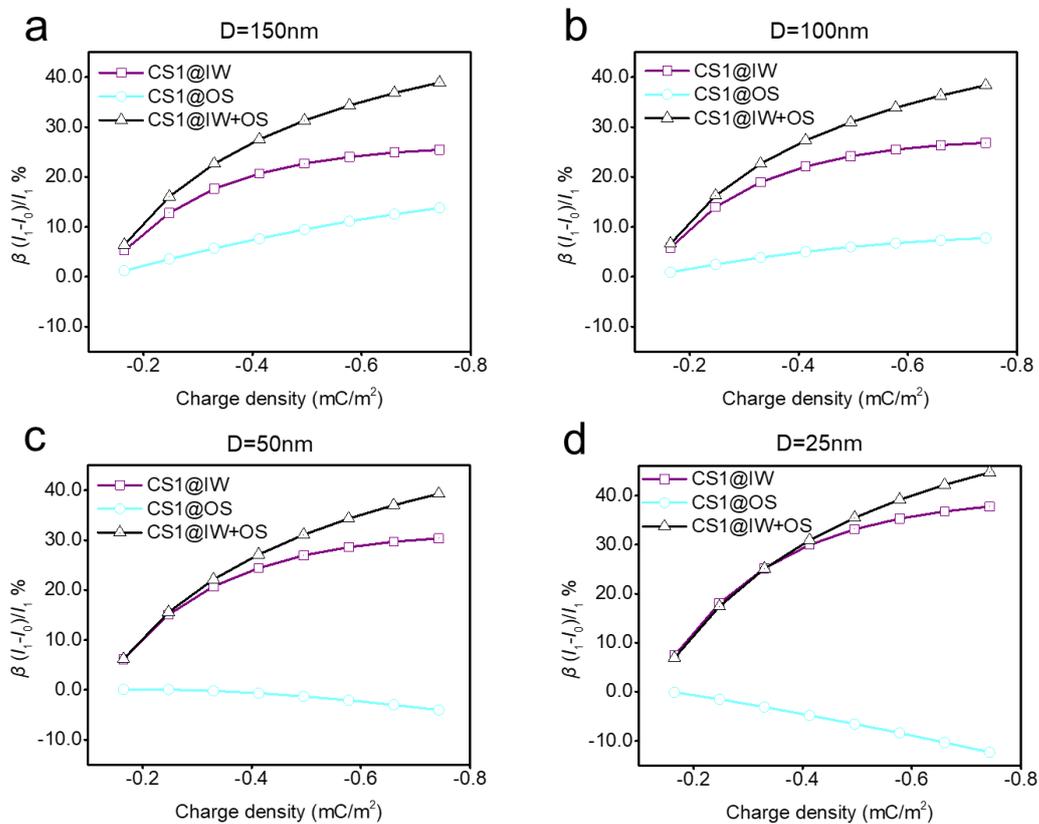


Figure S3. The effect of the base diameter of nanopore on the ion current signal. (a-d) The change ratio of ion current signal of different base diameter of nanopore with different surface charge.

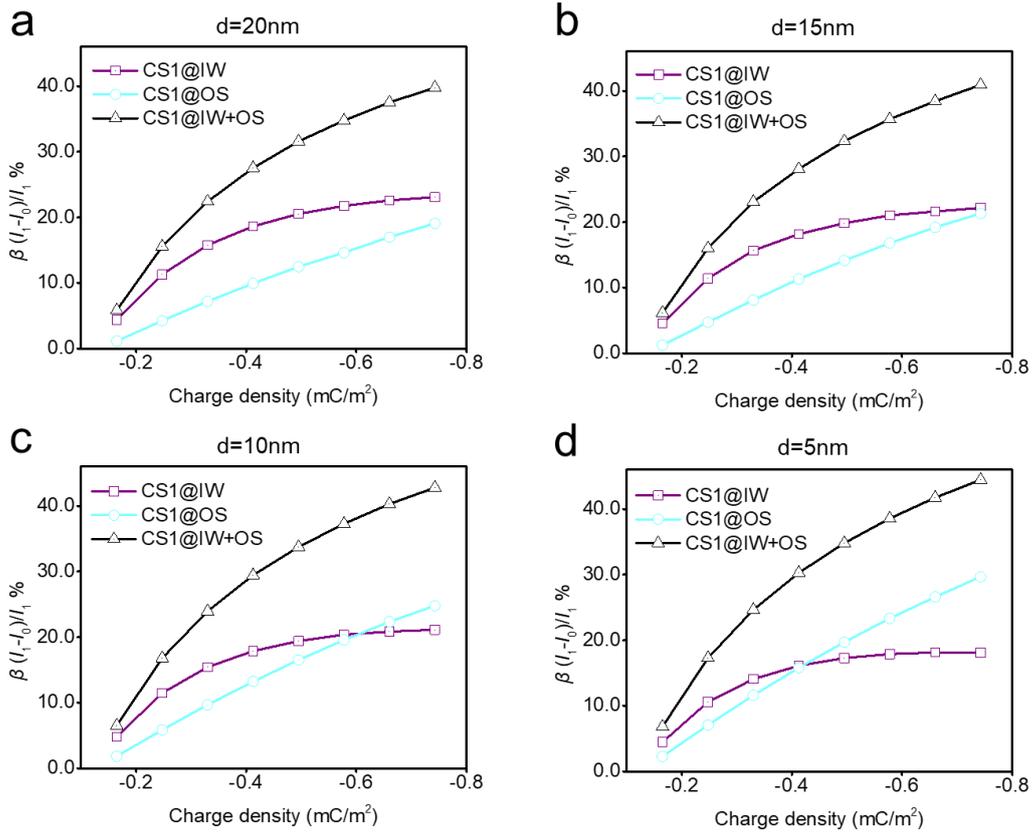


Figure S4. The effect of the tip diameter of nanopore on the ion current signal.(a-d) The change ratio of ion current signal of different tip diameter of nanopore with different surface charge.

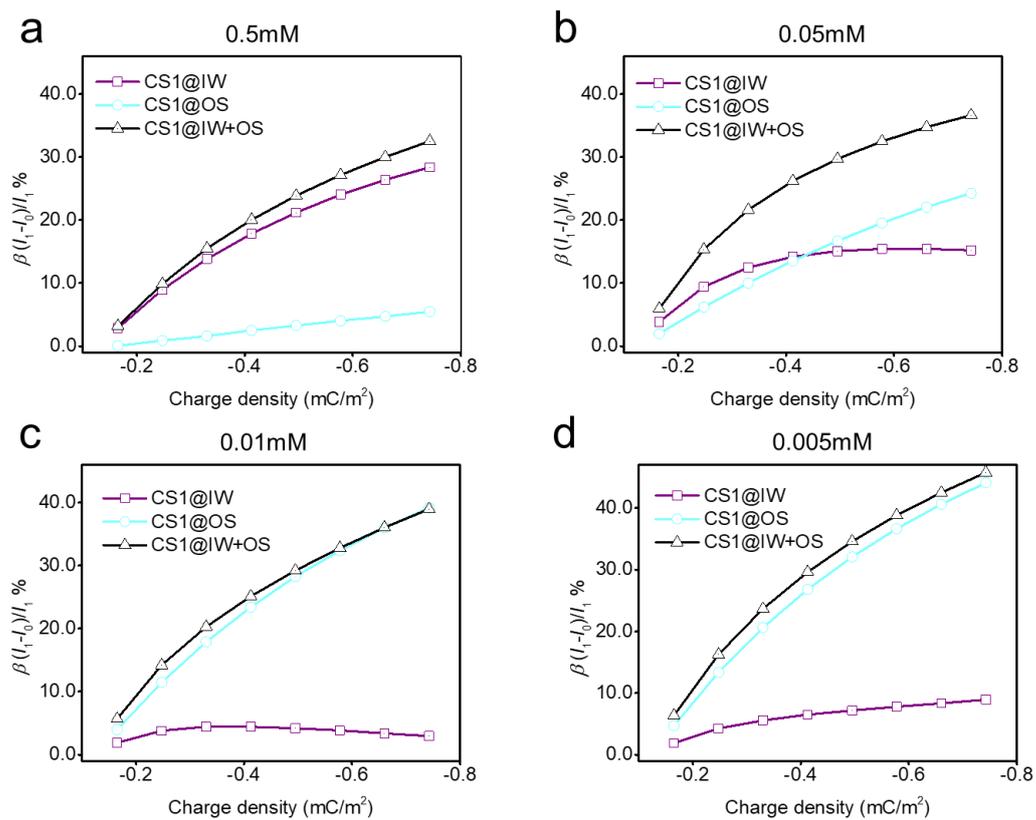


Figure S5. The effect of the ion strength of electrolyte on the ion current signal.(a-d) The change ratio of ion current signal with different the ion strength of electrolyte in different surface charge.

2. Supplementary Table

Table S1. Boundary conditions of surface charge density model and space charge density model.

Model	Boundary	Dilute Matter Transfer (Nernst-Planck Equation)	Electrostatic (Poisson Equation)
surface charge density model	1	$c(K^+) = c(Cl^-) = c_0$	$V_b V$
	2	$c(K^+) = c(Cl^-) = c_0$	$0 V$
	3, 4, 5, 6, 7, 8, 11, 12, 13, 14, 15, 16, 19, 20	$\vec{n} \cdot \vec{J}_i = 0$	Zero charge
	9, 10, 17, 18, 21, 22	$\vec{n} \cdot \vec{J}_i = 0$	$\vec{n} \cdot \nabla \varphi = -\frac{\sigma_s}{\varepsilon}$
space charge density model	1	$c(K^+) = c(Cl^-) = c_0$	$V_b V$
	2	$c(K^+) = c(Cl^-) = c_0$	$0 V$
	3, 4, 5, 6, 7, 8, 11, 12, 13, 14, 15, 16, 19, 20	$\vec{n} \cdot \vec{J}_i = 0$	Zero charge
	9, 10, 17, 18, 21, 22	$\vec{n} \cdot \vec{J}_i = 0$	σ'_s
	Nanoconfined space	—	$\nabla^2 \varphi = -\frac{\rho}{\varepsilon}$